

SYVAC3-CC4 USER MANUAL

NWMO TR-2011-22

June 2011

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Atomic Energy of Canada Limited

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ABSTRACT

Title: SYVAC3-CC4 User Manual
Report No.: NWMO TR-2011-22
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Company: Atomic Energy of Canada Limited
Date: June 2011

Abstract

CC4 (Canadian Concept generation 4) is a system model for the release and transport of radionuclides from a deep geologic repository. It includes a vault, a local geosphere, and the biosphere in the vicinity of any surface discharge zones. It is integrated with the SYVAC3 executive (System Variability Analysis Code) and the Modelling Algorithm Library (Version ML303) to form the reference Canadian postclosure safety assessment computer code. The version described here is SCC408, based on SYVAC3.12 and CC4.08.

The vault code simulates the following processes: random failure of containers through small defects; release of contaminants from UO₂ fuel, Zircaloy fuel sheaths, other metal wasteforms, or soft wasteforms to the interior of a failed container, including a radiolysis-based fuel dissolution model; precipitation of contaminants inside a failed container if solubility limits are exceeded, including calculation of solubility limits from groundwater composition for Np, Pu, Tc, Th and U; transport by diffusion of dissolved contaminants through the defect in the failed container to enter the surrounding buffer; transport by diffusion, advection and sorption of contaminants through the buffer, backfill and excavation damaged zone into the surrounding host rock using a nested-cylinder geometry; division of the vault into sectors, with release calculated from each sector into the local geosphere; and linear decay chains.

The geosphere model simulates the following processes: ability of the aquifer to provide water to a well; effect of the well pumping on the groundwater flow; diffusive and advective transport of contaminants in groundwater; converging and diverging flow paths; spatial variation in transport properties from segment to segment along the transport pathway, including linear equilibrium sorption and colloids; capture of contaminant plume by the well; and linear decay chains. The geosphere can have up to 10 unique states varying with time; for example, glaciation cycles. The geosphere transport can also be replaced by links to calculations conducted externally using, but not limited to, FRAC3DVS.

The biosphere model simulates the following processes: contaminant release into aquatic or terrestrial discharge zones; collection of all contaminants into a lake; concentrations of contaminant in the lake water, lake sediments, and in the surface soil of a garden, forage field, woodlot, and peat bog; contaminant concentrations in the air (indoor and outdoor); loss of radionuclides from the biosphere by radioactive decay, discharge from the lake, and burial into deep lake sediments; internal and external radiation exposures to members of a self-sufficient human household living in the area and using contaminated water, foods and materials; and internal and external radiation exposure to representative nonhuman biota. The biosphere model can contain up to four unique biospheric states, i.e. glaciation cycles (temperate, permafrost, ice sheet, and proglacial lake).

Mass accumulation and distribution is calculated in the models for the intact containers, failed containers, vault engineered barriers, geosphere and biosphere.

This manual describes the CC4 capabilities, limitations, execution, inputs and outputs, error and warning messages, and other information needed to run the model.

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1. INTRODUCTION

1.1 BRIEF OVERVIEW OF CC4 MODEL

CC4 (Canadian Concept version 4) is a system model for the release and transport of radionuclides from used nuclear fuel in a deep geologic repository. It includes the vault, geosphere and biosphere in the vicinity of the site. It is integrated with the SYVAC3 executive (System Variability Analysis Code) and the Modelling Algorithm Library (ML) to form the reference Canadian postclosure safety assessment computer code. The version described here is SCC408, based on ML3.03, SYVAC3.12 and CC4.08.

The CC4 vault model handles processes that occur in the wasteform, container, engineered barriers around an emplacement room, and the adjacent Excavation Damaged Zone in the near-field geosphere. It interfaces with a far-field geosphere by obtaining rock and groundwater properties from the geosphere model, and providing a contaminant release rate to the geosphere model.

The CC4 geosphere model is a model for contaminant transport from specified locations in the vault, to specified surface groundwater discharge locations, including a well. The geosphere model requires the pathways between these points to be provided from an external source, in the form of either a set of hydraulic heads at defined nodes or groundwater velocities for segments of the pathways. This transport path is then modelled as a set of 1-D transport segments or flow tubes that are connected together in 3-D space to form the transport network.

The CC4 biosphere model provides information on well depth and well pumping rate to the geosphere, and receives information on the radionuclide release rate to the biosphere from the geosphere. The biosphere model receives information from the geosphere on contaminant flows at defined discharge locations, and converts these flows to concentrations in the lake, air and soil. Ultimately, these contaminant concentrations are used to estimate dose to a self-sufficient human household living near the site and using contaminated water, food and materials. The model also estimates the dose rates to representative biota.

The theory behind the system model is described in more detail in the CC4 Theory report (NWMO, 2011).

1.2 CC4 SYSTEM MODEL REQUIREMENTS

1.2.1 Hardware and Software Requirements

The CC4 system model requires the SYVAC3 executive computer program. SYVAC3 provides common support functions for system models, notably input and output, single and multiple run management, probabilistic and deterministic sampling of input parameters, and robust numerical algorithms for generic time-dependent processes. More details on SYVAC3 are provided in the SYVAC3 Manual (Andres 2000).

CC4 is compliant with ANSI-standard FORTRAN 90, with some accepted residual features from Fortran 77 (e.g. use of EQUIVALENCE, use of nested IF constructs rather than CASE). The code does not use system level operating features, making it portable to a variety of

environments. The hardware platform must be capable of representing numbers between at least 10^{+38} and 10^{-38} . CC4 is capable of running as a batch file under Windows or Unix operating systems. Simulation time and disk space required depend on computer hardware (RAM, processor, network parameters if applicable, etc.) and simulation parameters such as simulation time limit, time series accuracy, number of compartments used for geosphere, number of climatic cycles in geosphere and biosphere, number of output files and time series written into the trace files. The hardware requirements for the CC408 median value simulation (SYVAC3-CC408) with 39 nuclides (4 chain and 8 single nuclides), a simulation time limit of 1.02×10^6 years that contained 100 glaciation periods, 10 compartments for each of 63 geospheric segments, a time series accuracy of 0.001 and basic output files, required approximately 1 hours 22 minutes and 200 MB of disk space on a 3 GHz Intel(r) Core(TM)2 Duo CPU E 6850 HP computer with 2.98 GB of memory. In comparison, the same simulation requires only ~3 minutes to run simulation with the same parameters with only one glaciation period (Temperate state) in the geosphere and biosphere over the whole length of the simulation.

1.2.2 User Requirements

In order to effectively utilize the CC4 system model, the user needs the following:

- A used fuel repository vault design;
- A description of the geosphere around the repository, including the likely contaminant transport paths (e.g. groundwater flow paths) between the repository and surface;
- The ability to prepare a geosphere mesh description compatible with the format requirements given in this report;
- A surface biosphere that characterizes the geosphere groundwater discharge locations, and has a surface water body to which the groundwater and surface runoff flow;
- A reference human group living near the repository, and characterization of its lifestyle habits, such as eating, that could expose it to contaminated food or materials;
- An understanding of the mechanisms for container failure and radionuclide release into the vault;
- An understanding of the equations and properties governing radionuclide transport through clays and geological media;
- An understanding of the equations and properties describing the pathways from contaminated water and soils to dose to humans and other biota;
- A user level understanding of the SYVAC3 code capabilities, limitations, and input/output file formats.

The modelling results are dependent on the input data used. The user is responsible for checking that the inputs are correct, and for evaluating the results for reasonableness. Defects in the CC4 code should be reported to the Nuclear Waste Management Organization (NWMO).

1.3 HISTORY OF THE CC4 MODEL

An earlier model, CC3, was developed by Atomic Energy of Canada Limited (AECL) for the 1994 postclosure safety assessment, which was presented to a Canadian Government Environmental Impact Assessment (EIS) panel. The CC4 system model was first used for the Second Case Study postclosure safety assessment (Goodwin et al., 1996). Table 1.1 summarizes the main features and differences of the two repository concepts modelled in the EIS and Second Case Studies, respectively. In these studies, CC3 and CC4 were used to estimate the average peak dose rate and time of peak dose rate to both human and non-human biota for these two repository concepts. They were also used for sensitivity studies.

CC4 is made up of the INROC (vault), GEONET (geosphere) and BIOTRAC2 (biosphere) submodels, which were combined under the SYVAC3 executive code. At the time of the Second Case Study, the code was labelled PR4, indicating that it was the prototype version of the present CC4 code. Subsequent to the completion of the Second Case Study, the review of the changes was completed and the system model was released as CC4.02. Subsequently, in CC4.03 the soil model was changed to a single surface soil compartment model, for greater transparency and consistency with other safety assessment models. CC4.04 was used as part of OPG's Third Case Study (TCS) project (Gierszewski et al. 2004). Version CC4.05 was used as part of OPG's Horizontal Borehole Case (HBC) Study project (Garisto et al. 2005). Version CC4.07 was used as part of a recent NWMO Glaciation Study project (Garisto et al. 2010). Some of the examples used in this User Manual are drawn from these studies, although they are not necessarily from the final reference cases.

1.4 DEFINITIONS

Acronyms used in this user manual are provided below:

AECL	Atomic Energy of Canada Limited
AWME	Analytical Well Model Equations
CC4	Canadian Concept generation 4
EDZ	Excavation Damaged Zone
EIS	Environmental Impact Assessment
HBC	Horizontal Borehole Case
NWMO	Nuclear Waste Management Organization
OPG	Ontario Power Generation Inc.
SYVAC3	System Variability Analysis Code generation 3
TCS	Third Case Study
TFE	Target Fractional Error

Table 1-1: Comparison of Selected Features of the EIS, Second, and Third Case Studies

	EIS Case Study	Second Case Study	Third Case Study
Emplacement option	In-floor	In-room	In-room
Vault depth	500 m	500 m	659 m
Number of fuel bundles	8.5 million	4.3 million	3.6 million
Vault area	3.2 km ²	3.4 km ²	1.8 km ²
Fuel burnup	685 GJ/kg U	720 GJ/kg U	792 GJ/kg U
Fuel cooling time	10 a	10 a	30 a
Number of bundles per container	72	72	324
Number of containers	118 700	60 100	11 232
Container shell material	Grade-2 Ti	high purity Cu	high purity Cu
Container corrosion mechanisms	Localized crevice and delayed hydride cracking	None	None
Fraction of containers failed instantly	10 ⁻³ to 10 ⁻⁴ (complete failure)	10 ⁻³ to 10 ⁻⁴ (pinhole failure)	2 x10 ⁻⁴ (pinhole failure)
Fraction of containers failed by 10 ⁴ a	1	10 ⁻³ to 10 ⁻⁴	2 x10 ⁻⁴
Effective buffer thickness	0.25 m	1.48 m	1.1 m
Effective backfill thickness	1.4 m	0.76 m	0.90 m
Rock permeability at vault depth	10 ⁻¹⁹ m ²	10 ⁻¹⁷ m ²	10 ⁻¹⁹ m ²
Rock porosity at vault depth	0.3%	0.001 to 0.1%	0.4%
Reference human group	Self-sufficient farm household	Self-sufficient farm household	Self-sufficient farm household
Well depth	Up to 200 m	Up to 100 m	Up to 100 m

2. FEATURES, CAPABILITIES AND LIMITATIONS

2.1 INTRODUCTION

The models are described in detail in the SYVAC3-CC4 Theory report (NWMO, 2011). The main features, capabilities and limitations of the model are briefly described in this section, according to Vault (Wasteform and Container), Vault (Engineered Barrier System), Geosphere and Biosphere.

2.2 PREDICTED VARIABLES

The main variables predicted by the various major submodels are summarized below.

Wasteform and Container

- The rate of flow of each contaminant out of the defect in a failed container.

Engineered Barriers

- The rate of flow of each radionuclide to each geosphere input location;
- The time of maximum release rate from each vault sector for each nuclide;
- The maximum release rate from each vault sector for each nuclide;
- The accumulated release from all vault sectors of each nuclide; and
- The number of failed containers in the vault.

Geosphere

- The rate of flow from each geosphere discharge location for each nuclide;
- The time of maximum flow from each geosphere discharge location for each nuclide;
- The maximum release rate from each geosphere discharge location for each nuclide;
- The maximum well capacity from the underground aquifer;
- The drawdowns in hydraulic head at nodes in the aquifer due to the well pumping; and
- The contaminant capture fractions by the well in the aquifer, which determine the quantities of contaminants entering the well.

Biosphere

- Maximum total dose over time to man from all exposure pathways and all nuclides;
- Time of maximum total dose rate;
- Maximum dose rate from all nuclides and all pathways up to a user specified time in years;
- Time of maximum dose rate from all nuclides and all pathways up to user specified time in years;
- Maximum dose rate for each individual nuclide and all pathways at the time of maximum total dose rate;
- Maximum dose rate for each individual nuclide up to simulation time limit;
- Time of maximum dose rate for each individual nuclide up to simulation time limit;
- Maximum dose for each nuclide and pathway;

- Maximum dose rate for each non-human biota type from all nuclides and all pathways up to simulation time limit;
- Time of maximum dose rate for each non-human biota type from all nuclides and all pathways up to simulation time limit;
- Maximum dose rate for each non-human biota type from all nuclides and all pathways up to specified time in years;
- Time of maximum dose rate for each non-human biota type from all nuclides and all pathways up to specified time in years;
- Maximum chemical element concentration for each element for six biosphere compartments up to simulation time limit;
- Time of maximum chemical element concentration for each element for six biosphere compartments up to simulation time limit;
- Maximum of the total radiotoxicity flux for all nuclides from the geosphere to the biosphere up to simulation time limit;
- Time of maximum of the total radiotoxicity flux for all nuclides from the geosphere to the biosphere up to simulation time limit;
- Maximum of the total radiotoxicity concentration for all nuclides in lake water up to simulation time limit, and
- Time of maximum of the total radiotoxicity concentration for all nuclides in lake water up to simulation time limit.

Mass Accumulation and Distribution

For the intact containers, failed containers, vault engineered barriers (buffer, backfill, and excavation damaged zone, EDZ), geosphere (all segments between (but excluding) the EDZ and the biosphere surface soil), and biosphere overall (surface water and degassing from soil and surface water), the following mass accumulation and distribution parameters are calculated for the above compartments:

- The remaining amount of nuclide in the compartment,
- The amount of nuclide lost to decay,
- The amount of nuclide formed by ingrowth in the compartment, and
- The amount of nuclide that flows out of the compartment.

2.3 WASTEFORM AND CONTAINER MODEL

The processes simulated are summarized below. These brief descriptions also indicate some of the main limitations of the model.

2.3.1 Geometry

The fuel geometry is neglected, except that a constant area is assumed in the fuel matrix dissolution rate calculation. The failed container water-filled interior is modelled as a well-mixed volume. The container defect is modelled as a small cylindrical hole through the container wall thickness.

2.3.2 Decay and Ingrowth

Since the nuclides decay at different rates, the relative inventories of the nuclides change with time and some nuclides decay into other nuclides. The inventory for all nuclides simulated is determined up to the simulation time limit for linear decay chains.

2.3.3 Container Failure

The assumed failure mechanism for the containers is through small holes in the outer container shell, e.g., from undetected fabrication defects, that permit the ingress of groundwater and the subsequent escape of nuclides. The time for this release to start is defined on a vault sector basis (i.e., same for any failed containers within a given vault sector). The number of failed containers in each vault sector is determined from the probability of defective containers that fail, the total number of containers in each sector, and a sector-dependent probability variable.

2.3.4 Wasteform Degradation and Nuclide Release

Release of nuclides from the wasteform is modelled by both congruent and instant release. The congruent release follows the wasteform degradation, which is modelled using one of four degradation methods; Radiolysis (used for UO_2 fuel only), Solubility Limited (currently used for degradation of the Zircaloy cladding), Constant Corrosion (used for metal wasteforms), and Rapid degradation (used for soft wasteforms).

The "instant-release" fractions of the nuclides are released from the wasteform to the interior of the failed container at the time the container is flooded with water (for the UO_2 fuel this is the portion of the inventory of each nuclide that is located in the gaps and at the grain boundaries of the fuel pellets). Congruent release refers to the release of nuclides that are uniformly immobilized in the wasteform host matrix. A nuclide is released as the matrix dissolves, at a rate that is proportional to the nuclide's abundance within the matrix and the rate of dissolution of the matrix. The nuclide's abundance depends on its inventory, modified to account for radioactive decay and exclusion of the instant-release inventory.

The Radiolysis based degradation method uses a set of empirical equations describing the dissolution rate of UO_2 fuel due to alpha, beta and gamma radiolysis of the surrounding groundwater. This degradation method is only applicable for the UO_2 fuel wasteform. The surface area of the UO_2 fuel wasteform is assumed to remain constant.

The Solubility Limited degradation method is based on the solubility of the wasteform and its loss rate from the container through the pinhole defect and ignores the initial transient. The Constant Corrosion degradation rate is constant from the time the container is flooded with water to the complete dissolution of the matrix. The Rapid degradation method uses a fixed (generally short) time, although this time frame need not be limited to any particular value, from the time the container is flooded with water to degrade the entire wasteform at a constant rate. If this time is very short, the release is equivalent to instant release.

The effect of groundwater composition on the degradation rates is not explicitly considered, other than through the conditions used to derive the solubility of some of the elements including the Uranium of the UO_2 fuel wasteform.

2.3.5 Precipitation

Some nuclides released from the fuel and clad to the interior of the container are relatively insoluble and precipitate. The input solubility limits can be used for all elements, but the vault model also allows the solubility limit of the five elements (neptunium, technetium, plutonium, thorium and uranium) to be calculated based on thermodynamic relationships and an input groundwater composition. If multiple isotopes of the same element are present in the same waste form, the elemental solubility limit is partitioned among the isotopes according to their relative abundance within the initial-and-as-decayed wasteform inventory. That is, the partitioning is based on the relative amount of each isotopes of that element within the same wasteform, allowing for decay and ingrowth with time, but not for any other loss mechanism from the wasteform.

Co-precipitation of isotopes is included by the partition of the shared solubility, but stable isotopes within the groundwater are not considered.

2.3.6 Release from Container

Nuclides released to the interior of a failed container and dissolved within the container water, are able to diffuse into the surrounding buffer through the container defect. The model determines whether transport out of the container is constrained by the resistance of the defect itself, or by diffusion into the surrounding medium, and uses the lower corresponding release rate. The container defect dimensions are kept constant.

2.4 ENGINEERED BARRIERS MODEL

The processes simulated are summarized below. These brief descriptions also indicate some of the main limitations of the model.

2.4.1 Model Geometry

The simplified geometry of the vault room is represented as shown in Figure 2.1. The user must determine the dimensions in the model that best approximate the physical room geometry (e.g., same volume, or same radial thickness), especially for in floor placement geometries.

Each room is approximated as a cylindrically nested concentric series of layers of buffer, backfill, excavation damaged zone (EDZ), and the geosphere near-field rock. The near-field rock is modelled as semi-infinite. All properties are assumed to be symmetric about the cylindrical axis. Since actual disposal geometries are unlikely to have this cylindrical symmetry, equivalent radii must be chosen as inputs.

A finite axial extent is considered, corresponding to the room length. The contaminant source is modelled as a point source located along the central axis. The model is not sensitive to its axial position.

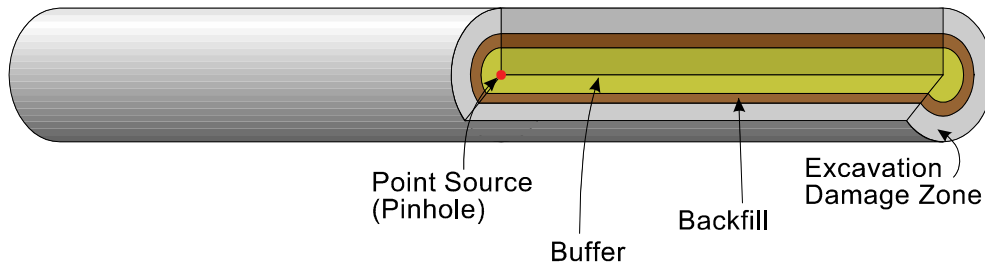


Figure 2.1: Emplacement Room Model Geometry

2.4.2 Groundwater Flow Through Vault

Permeability in the buffer is taken to be small, so there is no groundwater flow. However, groundwater velocities are modelled in the backfill, EDZ and surrounding rock. In these media, each sector has a uniform radial and axial flow. The groundwater flow rates in the rock are taken from the values supplied by the geosphere model. The backfill and EDZ flow components are calculated by a Darcy's law (Johnson et al. 1996).

The actual groundwater flow within the vault would not be radial, but an effective radial flow rate within the buffer and backfill is estimated based on the rock groundwater flow orthogonal to the room axis. The groundwater flow should be compared with results from a more detailed model such as a finite-element model, to determine the level of agreement. For example, comparison with finite-element solutions to the 3-dimensional convection-dispersion equations shows agreement within a factor of two in integrated flows out of the vault for conditions similar to those in the Second Case Study (Johnson et al. 1996).

2.4.3 Transport Through Buffer, Backfill and EDZ

The release rate from the failed container calculated in the Wasteform/Container model is taken as the input source term. The model assumes azimuthal symmetry around each room. It solves the radial transport equations exactly, and models the axial transport approximately (it is solved accurately within each layer, but uses an integrated boundary condition between layers). A convective type boundary condition for contaminant transport is imposed in the axial ends of the vault sector (i.e. no diffusive transport).

Since the buffer is impermeable, contaminants move only by diffusive transport. However, groundwater velocities could be significant in the backfill, EDZ and surrounding rock. In these media, contaminants can move by advection, dispersion, and diffusion. Diffusion constants in the buffer, backfill, EDZ and geosphere vary by element. Diffusion coefficients do not change with time.

Release rates of contaminants are integrated over the entire surface of the EDZ for each sector (mol/a). Concentrations of the contaminants in the porewater are not determined.

2.4.4 Sorption

Each contaminant interacts with the solid phase (buffer, backfill, EDZ, geosphere) by linear equilibrium sorption. Non-linear sorption and saturation of sorption sites are not modelled.

2.4.5 Decay Chains

Transport is modelled for linear decay chains.

2.4.6 Resaturation

The vault re-saturation phase is not modelled. It is assumed to be fully saturated by the start of the nuclide release calculations in each sector. No fluid phase changes, such as water to steam or to ice, are allowed. The model assumes that the Eh conditions are constant throughout the vault – i.e., consistent reducing (or oxidizing) parameter values should be used.

2.5 GEOSPHERE MODEL

The processes simulated are summarized below. These brief descriptions also indicate some of the main limitations of the model.

2.5.1 Geosphere Groundwater Flow

In the geosphere, the groundwater flow is not directly calculated, but rather must be determined externally to CC4 and used to define a three-dimensional (3-D) description of the transport pathways of contaminants, which is input to the model as a mesh or network of nodes and segments.

2.5.2 Geosphere Transport Network

The transport segments of the geosphere network are placed to coincide with the pathways that contaminants would follow as they move from the vault to the biosphere, as determined by external groundwater flow and transport simulations, typically using detailed models such as MOTIF or FRAC3DVS. Figure 2.2 provides an example geosphere network.

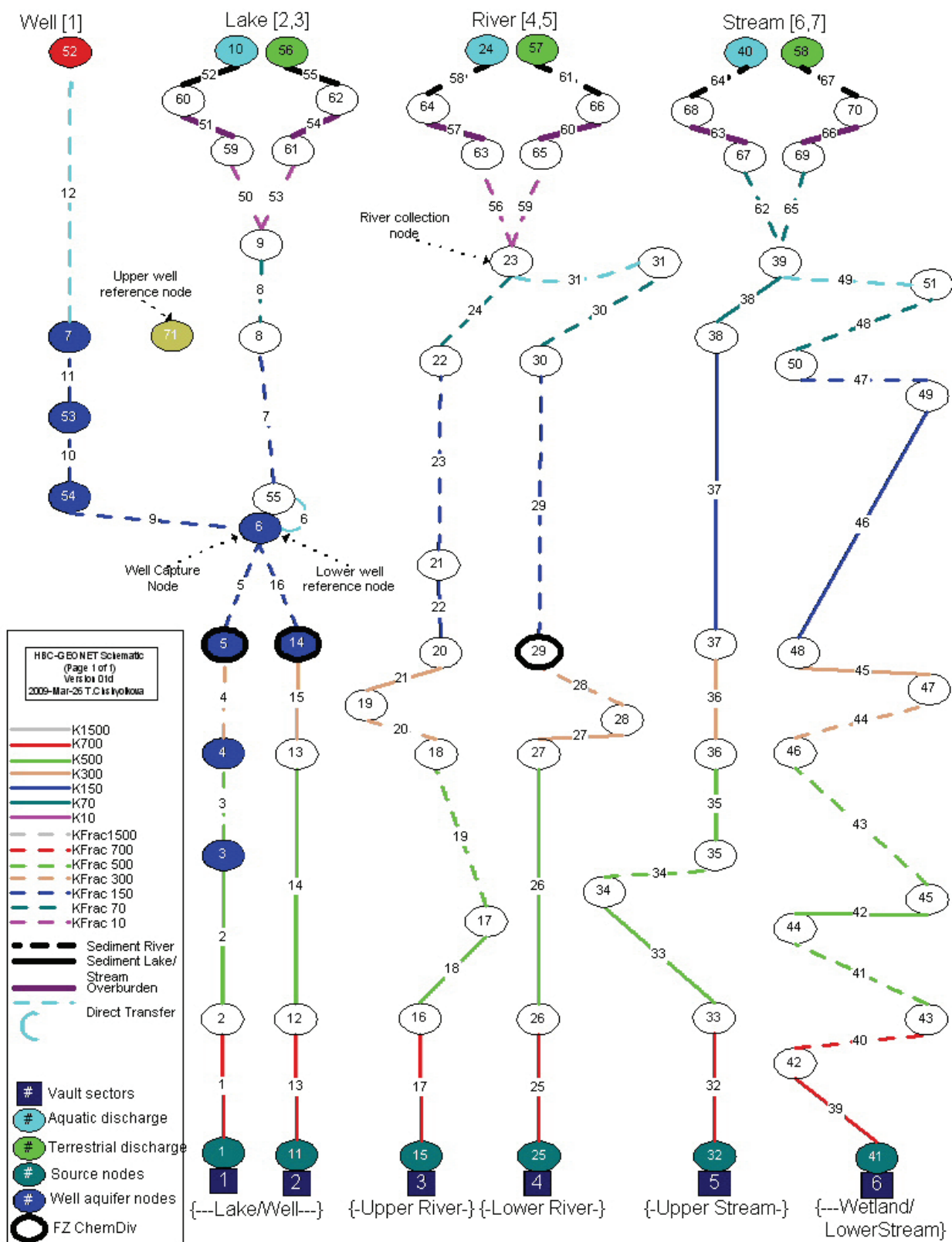


Figure 2.2: Example Schematic of the Geosphere Network

Note that groundwater flow alone does not necessarily indicate the transport paths if contaminant transport is dominated by diffusion rather than by groundwater advection. In such cases, the geosphere transport network segments should be along the lines of maximum concentration gradient, representing the shortest diffusion paths to regions where the permeability and groundwater flow are significantly higher.

The network incorporates the hydro-geological stratigraphy and geological structures, the geochemistry of the rock and the groundwater, and the groundwater flow field. The contaminant flow out from one segment of the network is calculated and used as the input to the next segment of the network. The transport network may converge (additive) and diverge, (diverging fractions defined in the input file or calculated as a result of changing operation of the well).

The positions of nodes in the geosphere are represented in Cartesian coordinates defined in the main input file, relative to an arbitrary origin, with the positive z direction as vertical. The connectivity of the nodes defines the positions of transport segments. The order of node calculations is automatically determined based on information in the geosphere network file.

The characteristics of each transport segment that are input are: equivalent porosity; tortuosity; and mineral composition (segment average values). It is possible to define the groundwater flow by specifying either hydraulic head and permeability (or hydraulic conductivity) data, or by specifying groundwater flow rates directly.

2.5.3 Superposition of Well

A groundwater supply well can be defined in the geosphere transport network by a set of nine nodes in models where a well is specified. Two of the nodes are reference nodes, which may or may not be a part of the transport network, and which define the orientation and position of the central groundwater flow line to the well. The other nodes are part of the transport network. One node, the well discharge node, is located at the ground surface and the other nodes are located in the aquifer from which the well draws its water. One of these nodes is the actual well node in the aquifer; the other two, called drawdown nodes, define two short segments leading to the well and are placed at specified distances from the well node in the aquifer. These two drawdown nodes are used to represent the shape of the hydraulic head drawdown created near the well by pumping. This set of well nodes is connected to the rest of the transport network through one or more well capture nodes that collect the contaminants moving from other parts of the network and lead them to the well. The positions of these nodes (the well discharge node, the well node in the aquifer, and the drawdown nodes) are adjusted automatically by CC4 to give the user-input well depth (i.e., the vertical distance between the well node at the surface and the node representing the intersection of the well with the aquifer). The well node in the aquifer is moved along the central flow line and the well discharge node is located at the ground surface vertically above.

2.5.4 Drawdowns in the Aquifer due to Well

The effect of the well is to perturb the reference groundwater flow field in the aquifer containing the well. This is modelled by adjusting the hydraulic head at the position of each node in the aquifer containing the well using the Analytical Well Model Equations (AWME) described in the CC4 Theory Manual. The groundwater velocities are recalculated once the head drawdowns have been determined.

Wells that are not deeper than the bottom of the overburden layer are classed as overburden wells. Overburden is specified in the model at all areas where transport pathways from the vault discharge to the biosphere, including the well discharge. The model assumes that such wells draw no water from the groundwater aquifer, but rather are supplied entirely from surface waters which are contaminated at the same concentration as the lake water.

2.5.5 Maximum Well Capacity

A maximum well capacity is defined from the AWME based on the properties of the aquifer. This value is provided to the biosphere model, which then determines the actual demand placed on the well. This demand is a constant annual amount.

If the well demand is larger than can be supplied by deep groundwater flowing in the aquifer, then the additional water is assumed to be supplied by surface waters captured due to the well drawdown, leading to a dilution in the well water contaminant concentration. This pathway from surface to well is not modelled in the transport segments.

2.5.6 Plume Capture Fractions

One or more nodes of the transport network are considered to be well capture nodes. These nodes are placed on a capture line oriented orthogonal to the central flow line passing through the well. This line is located at a distance farther down the dipping aquifer than the deepest well nodes. The segments leading from these capture nodes to the first well drawdown node (the well collection node) are assigned widths that represent the widths at the capture line. The envelope of these widths represents the total width of the contaminant plume at this point.

The fraction of contaminants from the vault moving along pathways in the aquifer that is captured by the well is determined from the stream function expression given by the AWME. The fraction of the contaminants captured by the well is transported to the well drawdown nodes and then to the well itself. The drawdown nodes are used to give better definition to the drawdown cone in the aquifer in the region near the well. The fraction of the contaminants not captured by the well is transported along well bypass segments to other network nodes for eventual discharge at the ground surface.

The well model assumes that pumping is from a confined aquifer with constant and uniform hydraulic properties. The well is also assumed to be located over the centre of the plume and near a constant hydraulic head boundary (for example, a lake), located where the aquifer comes to surface.

2.5.7 Hydrodynamic Dispersion Coefficient

A longitudinal hydrodynamic dispersion coefficient for each nuclide in each transport segment of the network is determined from the sum of a mechanical dispersion term and an effective diffusion term.

The transport solution for nuclides in decay chains uses a single dispersion coefficient in each segment that applies to all nuclides in the chain; the value determined for the first member of the chain is used for all chain members. When the mechanical dispersion term dominates the dispersion, the dispersion coefficient has the same value for all chain members anyway. When the diffusion term dominates, the diffusion coefficient for the first chain element will be used.

However for the actinide elements in decay chains, Am, Np, Pa, Pu, Ra, Th, and U, the diffusion coefficients have about the same value, and so using a single value for dispersion coefficient for all members of a decay chain is a good approximation.

2.5.8 Groundwater Velocity

Average linear groundwater velocities for each segment are determined by one of six possible methods:

- Average linear velocities supplied directly as input for each segment.
- Specific discharges (Darcy velocities) supplied for each segment. Average linear groundwater velocities are then calculated from segment porosity.
- Reference hydraulic heads supplied for each node, and hydraulic conductivities supplied for each segment. Average linear groundwater velocities for each segment are then calculated in the network model from Darcy's law.
- Reference hydraulic heads supplied for each node and intrinsic permeabilities supplied for each segment. Hydraulic conductivities determined from reference properties of water and average linear groundwater velocities for each segment are calculated as above from Darcy's law.
- Reference hydraulic heads and temperatures supplied for each node and intrinsic permeabilities supplied for each segment. Hydraulic conductivities determined from variable properties of water as a function of temperature and pressure due to depth. Average linear groundwater velocities for each segment are calculated as above from Darcy's law.
- Reference hydraulic heads and temperatures supplied for each node, and intrinsic permeabilities supplied for each segment. Hydraulic conductivities determined from variable properties of water as a function of temperature and pressure due to depth. Average linear groundwater velocities for each segment are calculated from an enhanced version of Darcy's law that includes the effects of buoyancy when there are variations in the density of the groundwater. In this case, the reference hydraulic heads supplied must be determined from detailed groundwater flow modelling that also includes the buoyancy effects.

2.5.9 Spatial Variation of Transport Parameters

Each segment of the transport network is assigned constant physical and chemical properties. However, transport properties can vary from segment to segment along the transport pathway. The details of the site model should define the appropriate size and spacing of the segments to reflect the spatial variation in these properties.

2.5.10 Retardation Factors

Retardation factors are calculated using empirical equations, depending on a set of location-specific chemical and mineralogical properties that are defined for each transport segment. A set of element/mineral-specific distribution coefficients has been developed to relate these specific properties of the transport paths to the amount of retardation that can occur.

In particular, the overall retardation factor R for a given nuclide and transport segment (in the geosphere) is:

$$R = 1 + \sum_m f_m (vK_d)_m$$

where K_d is the (measured) sorption coefficient on a given mineral m , and $(vK_d)_m$ provides for the scaling from the measurement conditions to the conditions of interest here, and f_m is the fractional abundance of each mineral in the segment. Typically K_d values are measured in high-porosity crushed rock column experiments, and so the recommended transformation to retardation in low-porosity solid rock settings is $(\rho K_d/\varepsilon)$, where ρ is the solid mineral density and ε is the porosity of the experimental setting for the given value of K_d .

A simple switch between oxidizing and reducing conditions is used. The location along the flow path, where the redox potential E_h switches over from reducing to oxidizing, is determined by the depth of a redox divide. Segments lying below the divide are considered to be reducing; segments lying above the divide are considered to be oxidizing. The switching point for determining if a segment is above or below the divide is the depth at the mid point of the segment.

2.5.11 Other Site-Specific Effects of the Well

The Analytical Well Model (AWME) is used for flow within the aquifer and is generic (not site-specific). Depending on the site-specifics, the well may also affect:

- The drawdowns outside of the aquifer (drawdowns in the aquifer are determined by the analytical well model);
- Changes to discharge areas at the biosphere interface; and
- Capture fractions for segments leading to the well from outside the aquifer.

Any equations that apply to these quantities for use in the geosphere model are contained in the module SSPWEL.FOR (Site-Specific Well Effects). In SCC408, the site-specific effects are:

- determination of drawdown outside aquifer,
- modified discharge area at discharges to biosphere, and
- well capture fractions (fractionation of flow at divergence points) at nodes outside the well aquifer.

2.5.12 Converging and Diverging Flow Paths

A schematic example of a transport network is shown in Figure 2.2. Transport segments can either converge or diverge at nodes, and they connect together to represent the transport pathways leading from a source of contaminants to discharge locations in the biosphere. If segments converge, their output is summed before being used as input to the succeeding segment. If segments diverge, the output of a segment is fractionated, and a portion is used as input to each succeeding segment.

2.5.13 Matrix Diffusion

Matrix diffusion is the process whereby solutes that are being transported in moving groundwater diffuse into adjacent stagnant water in the rock matrix. A value for the effective

fracture aperture that is $>1 \mu\text{m}$ is used as a switch that determines whether matrix diffusion is invoked as a transport process. Presently, matrix diffusion, when invoked, is treated by adjusting the retardation factor and dispersion coefficient. However, this approach only provides an approximation of the effects of matrix diffusion, which would need transport calculations in at least 2 dimensions to treat more exactly.

2.5.14 Surface Discharge

The geosphere model supports five surface discharge types: WELL, AQUAtic, TERRestial, BOG (wetland), and GASEous discharge. However, it does not do anything with this information other than pass it on to the biosphere model. The geosphere model also accepts a GASEous input, in addition to the AQUAtic input, from the vault model for propagation to the discharges to the biosphere.

2.5.15 Segment Boundary Conditions

The transport along each segment is determined using convolution integrals and response functions. These solutions are available for the following segment outlet boundary conditions: semi-infinite medium, mass transfer coefficient, zero concentration, and source within medium.

Note that the transport along the segments is solved sequentially in an order specified by the user, so that other than the boundary conditions, each segment is not affected by the conditions in a downstream segment. However the conservation of water conditions (continuity of specific discharge) built into the groundwater flow field supplied means the propagation of groundwater flow conditions from segment to segment is taken care of.

2.5.16 Geosphere/Biosphere Interface

The principal interface between the geosphere and biosphere models is the passing of the time-dependent flow rates of contaminants from the vault at each of the discharges to the biosphere.

In addition, the aquatic and wetland (bog) discharge nodes have two extra nodes assigned by CC4 - a sediment node and an overburden node, as shown schematically in Figure 2.2. The properties of these layers can be significantly different from the bedrock, and therefore significantly affect transport of some nuclides, even though they may be comparatively thin. The two nodes define the positions of the bottom of these layers at these discharge locations. CC4 reduces the thickness of the last bedrock segment by the thickness of these layers. Note that these layers can have zero thickness. Terrestrial discharge zones usually have an overburden layer only, although a layer of saturated soil, analogous to sediment at an aquatic discharge, could also be introduced.

The geosphere model passes porosities and sorption distribution coefficients for the sediment layers and also passes the retardation factors for the last segment of the pathway leading to each groundwater discharge area to the biosphere model. For most aquatic discharge locations this last segment will be the segment passing through the sediment layer; for the discharge into a well, this segment is the last segment in the aquifer from which the well water is drawn; for terrestrial discharges, this last segment is generally the segment passing through the overburden layer. These retardation factors are used for calculations of nuclide mass flow rates out of the geosphere for daughters in secular equilibrium with their parent nuclides.

The maximum well capacity obtained from the analytical well model is passed to the biosphere model for use in determining the possible well uses. Subsequently, the actual pumping demand placed on the well is determined by the biosphere model, and the well demand is passed back to the geosphere model.

2.5.17 Colloids

The model considers reversible sorption of the contaminant onto the colloids, composed of a single colloid mineral. The colloid itself may migrate more slowly than the groundwater. The effects of colloids are applied as modification in the retardation factor equations used in the geosphere transport equations.

2.5.18 FRAC3DVS Data Usage

Data from the code FRAC3DVS may be used instead of the CC4 calculated geosphere flows from the geosphere model. One control file and one or more data files must be present in the same run directory in order for FRAC3DVS data to be used. The control file provides information for the FRAC3DVS data file names along with nuclide names and a cross references to the FRAC3DVS slice label and CC4 discharge locations which are to use the FRAC3DVS data. Once a control file is detected in the run directory, the data from the FRAC3DVS data files are read and geosphere flow time series are created, overwriting any CC4 calculated geosphere flows for that simulation. FRAC3DVS data is only provided for one simulation so if a probabilistic simulation is requested only the first simulation will use the FRAC3DVS data and the rest of the simulations will use the CC4 calculated geosphere flows.

For more information on the FRAC3DVS control input file format and the FRAC3DVS data file format see Section 5.2 and Appendix L.

2.6 BIOSPHERE MODEL

The processes simulated are summarized below. These brief descriptions also indicate some of the main limitations of the model. Figure 2.3 illustrates the biosphere landscape.

2.6.1 Concentrations in Surface (Lake) Water

The surface biosphere is modelled as collecting into one surface body, nominally modelled as a lake. The lake is modelled as well mixed, with a defined outlet discharge rate which constitutes one of the four contaminant loss routes from the model (the others are the deep lake sediment, radioactive decay, and gaseous evasion from the lake).

The entire contaminant discharge is assumed to end up in this lake, with negligible delay after discharge. Small fractions of the discharges may be held up in the soil zone before reaching the lake. However, it is conservatively assumed that this fraction is small. The amounts thus diverted from entering the lake are not subtracted from the discharge flows to the lake, and no decay due to its time delay is considered.

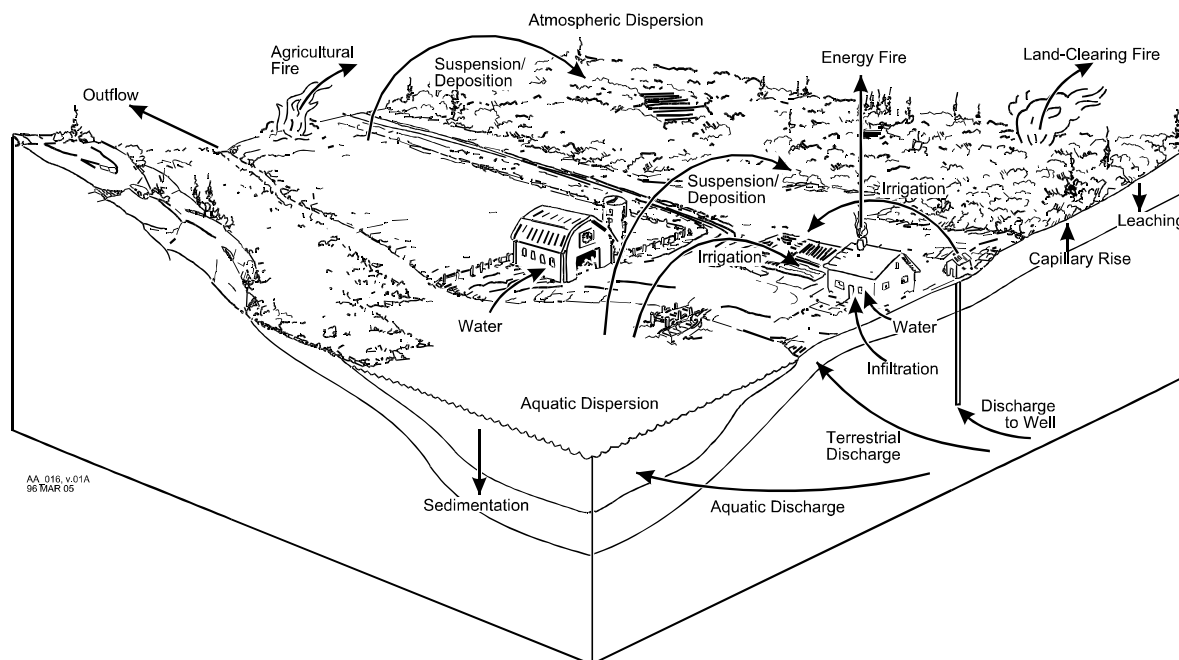


Figure 2.3: Conceptual Landscape of the Second Case Study Biosphere

2.6.2 Concentrations in Lake Sediment

The aquatic discharge zones (into the lake bottom) are covered by a layer of mixed and biologically active sediment, lying on a compacted deep layer. Contaminants are continuously removed from the lake water by sorption on suspended particles and deposition in sediments.

This sedimentation occurs continuously and contributes to sediment bulk at the bottom of the lake.

2.6.3 Concentrations in Surface Soil

The soil model calculates the concentration of each nuclide in the soil of the rooting zone in the four field types that may be used by the reference human group. The soil concentration considers both contamination from atmospheric deposition and from irrigation, as well as from contaminated groundwater that rises up through the soil to the surface.

The fields are located over the terrestrial parts of the discharge zones in a manner that maximizes the potential human exposure to contaminants. If soil is organic and peat is burned for energy, the field order is peat bog, garden, forage field, and woodlot. If the soil type is not organic, then peat bog is not used and the order is garden, forage field and woodlot. The fields differ in probabilities of irrigation and their source of irrigation (if any).

2.6.4 Use of Sediments in Fields

In some simulations, the fields are assumed to lie as much as is physically possible on fresh sediments, either because the lake was recently drained for farming, or the sediments were dredged for use on the fields. Each discharge covers an area on the lakebed. Any areas of the lakebed not over a discharge are assumed to be covered by sediments with the same nuclide concentration as the mixed sediment layer. The terrestrial fractions of the discharges are usually small and are not included in the calculation. The fields (possibly in several portions) are assumed to lie over the discharges. The resulting soil concentration in each field consists of an area-weighted average.

2.6.5 Concentrations in Atmosphere

The atmosphere model calculates nuclide concentrations in air due to suspension of particulates and gases from soils, vegetation and the lake. Noble gases are modelled separately.

For some sources, an empirical dispersion effect is included, but not for all. No radioactive decay or ingrowth is accounted for in the atmosphere. The loss of contaminant from soil to the air does not reduce the contaminant levels in the soil, and similarly the deposition of contaminants from the air is assumed not to reduce the contaminant levels in the air. These processes are essentially considered to either balance or be small effects that can conservatively be ignored.

2.6.6 Deposition to Soil and Vegetation

The soil can only receive additional radionuclides from either irrigation water or atmospheric input that originates from the surface water body (lake).

Vegetation is assumed to receive radionuclides from the atmosphere that have originated from all sources. This is conservative in the case of fires where the vegetation is burned, but then a portion of the radionuclide inventory is redeposited.

2.6.7 Internal and External Radiation Exposure for Humans

The food-chain model and related dose pathways used for the determination of the internal and external radiation exposure for the reference human groups is expressed as a multiplier of the contaminant concentration in water, soil or atmosphere via transfer factors. The resulting food and media concentrations are then translated into a radiological dose to man.

2.6.8 Internal and External Radiation Exposure for Nonhuman Biota

CC4 estimates the dose rate for a generic mammal, bird, fish and plant, using similar but fewer dose pathways than are used for humans.

2.7 GLACIATION SCENARIO

The ability to represent time dependent geosphere and biosphere states was added to the SYVAC3-CC4 code in version CC4.07. In this section the glaciation scenario will be used as an example of how state dependent geosphere and biosphere states can be used. However, it should be noted that this capability is generic and can be used to represent state dependent parameters unrelated to glaciation. The glaciation scenario was implemented for the geosphere and biosphere models only as the assumption is the effects of glaciation may not reach the vault. The geosphere uses the multi-compartment model for glaciation. The biosphere uses data changes to simulate various biosphere states.

2.7.1 Glaciation Scenario in the geosphere

To model glaciation in the geosphere, the multi-compartment model is used for certain segments, particularly for those closer to the surface and affected by permafrost. The multi-compartment model includes an extra compartment to act as a boundary for the segment, at which the boundary condition can be applied. Two response functions, #5 and #6, are implemented using the multi-compartment model. The boundary compartment for response function #5 is given the same properties as the other sub-compartments, thus acting as if the current segment extends further, analogous to the semi-infinite medium response function, #1. Response function #6 is similar but implements a zero concentration boundary, analogous to response function, #3. These response functions are set in the fixed geosphere network data file.

The number of compartments used in the transport segment can be set in the sampled input parameter DCMPT in the main input file. This parameter should have a maximum value of MXCOMP-2 otherwise it is reset to MXCOMP. The user must increase MXCOMP and recompile if a larger number of compartments are needed.

There can be up to 10 unique periods or states in the geosphere (MXGSTA), mainly referring to groundwater flow conditions. These states can repeat over and over during a glaciation cycle or series of cycles.

With several cycles through the glaciation periods, the time series output may need to be adjusted to more accurately represent the time series. This can be achieved by resetting the maximum number of time points in a time series in the time series control section of the input file.

2.7.2 Glaciation Scenario in the biosphere

To model glaciation in the biosphere, different data values are used to represent different biosphere periods. There can be up to 4 unique states in the biosphere (MXBSTA), which are associated with a critical group: temperate – farmer, permafrost – hunter, ice sheet –no biota, proglacial lake – fisherman. These states can repeat over and over during a glaciation cycle or series of cycles.

2.7.3 Cross reference indices from periods to states

The cross reference index from periods to states for geosphere (GIDXS) helps to determine the period for the geosphere during each of the 100 states. Similarly, the cross reference index

from periods to states for the biosphere (BIDXS) establishes biospheric state during each of the 100 (MAXPER) periods. Both parameters have dimension of MAXPER.

2.8 OTHER RESTRICTIONS AND CAUTIONS

Other general restrictions related to the use of the SYVAC3-CC4 code are noted below.

2.8.1 Numerical Stability

The transport models are semi-analytical, and as such do not suffer from spatial discretization errors commonly associated with numerical solution methods such as finite elements. Time dependence is solved using a response function based approach that also does not depend on the accuracy of the solution at earlier times. Numerical analysis involves notably evaluation of response functions, numerical integration, and inversion of Laplace transforms. These are solved by the vault model or SYVAC3 routines that have been shown to be robust for conditions similar to the Second Case Study (Goodwin et al. 1996).

2.8.2 Numerical Accuracy

The vault boundary-integral transport solution has been designed to be accurate to close to machine precision, and in general will exceed the accuracy, to which the input data are known.

Error estimates are made for the numerical Laplace inversion, and warning messages provided if needed.

The representation of a time-dependent result by a time series (a set of finite time points) results in some interpolation error when combining time-series. Time-series may have large local errors where absolute values are relatively small. Time series accuracy can be improved through the input file by judicious choice of the time series smoothing parameter values, by defining required time points where important results are expected, by increasing the allowed number of time points per series, and by reducing the target fractional error in creating a time series.

Time series may accumulate errors when numerous small time series are added onto a few significant time series; e.g. in calculating total dose as a sum of individual nuclide dose rates. This shows as a "waterfall" shaped time series profile at the fixed time points. It can be minimized by ordering the nuclides in the chain list such that the most significant nuclides to total dose are calculated later.

The decay chain inventory solution may not be accurate if the half-lives range over more than a factor of 10^{13} , but for real decay chains has been found to be accurate to within 0.2%.

2.9 DEFAULT PARAMETERS

2.9.1 Fixed Parameters

Default parameters are defined through PARAMETER statements in the INCLUDE files, and can be changed by recompiling the code. The main default parameters are as follows:

- AVOGAD = 6.022045×10^{23} , Avogadro's number [mol^{-1}];
- GRAVAC = 9.807, acceleration due to gravity [m/s^2];
- MNHLIF = 0.0027, minimum half-life [a]
- MXHLIF = 1.0×10^{30} , maximum half-life for calculations, otherwise decay constant set to zero [a];
- PI = 3.141592653589793;
- T273K = reference temperature of 273.15 K [K];
- TDELTA = 0.01, duration of short time pulse, typically used for modelling pulse input of material into a compartment [a];
- CFDPA = 3.652422×10^2 days per annum [d/a];
- CFM3PL = 1.0×10^{-3} value cubic metres per litre [m^3/L];
- CFSPA = 3.1556926×10^7 seconds per annum [s/a];
- CFSPD = 8.64×10^4 seconds per day [s/d];
- RADLYS = 1 index used to identify radiolysis degradation method;
- SOLLIM = 2 index used to identify solubility degradation method;
- CNSTCR = 3 index used to identify corrosion rate degradation method;
- INSRLS = 4 index used to identify instant release degradation method;
- NHMAML = 1 index used to identify a non-human biota;
- NHBIRD = 2 index used to identify a non-human biota;
- NHPLNT = 3 index used to identify a non-human biota;
- NHFISH = 4 index used to identify a non-human biota;
- MAMLNH = 5 index used to identify the mammal in the terrestrial animal types;
- BIRDNH = 6 index used to identify the bird in the terrestrial animal types;
- PLNTNH = 7 index used to identify the plant in the terrestrial animal types;
- MEAT = 1 index used to identify one of the three terrestrial animal food types;
- MILK = 2 index used to identify one of the three terrestrial animal food type;
- BIRD = 3 index used to identify one of the three terrestrial animal food types;
- PLANT = 4 index used to identify the plant food type in the food chain;
- FISH = 5 index used to identify the fish food type;
- NONE = 0 index used to identify no source for irrigation water;
- LAKE = 1 index used to identify the lake as source of water;
- WELL = 2 index used to identify the well as source of water;
- ATMOS = 3 index used to identify a source of deposition;
- SAND = 1 index used to identify a type of soil;
- LOAM = 2 index used to identify a type of soil;
- CLAY = 3 index used to identify a type of soil;
- ORGANC = 4 index used to identify a type of soil;
- FORAGE = 1 index used to identify the forage field, a field type;
- VEGPCH = 2 index used to identify the vegetable patch (garden), a field type;
- WOODLT = 3 index used to identify the woodlot, a field type;

- PEATBG = 4 index used to identify the peat bog (wetland), a field type;
- AGRIFR = 1 index used to identify agricultural fires;
- LANDFR = 2 index used to identify land clearing fires;
- ENERFR = 3 index used to identify energy fires;
- INORG = 1 index for inorganic building material; and
- WOODEN = 2 index for wooden building material.

2.9.2 Maximum Array Dimensions

Array dimensions are defined through PARAMETER statements in the INCLUDE files, and can be changed by recompiling the code. The main default dimensions applicable to SYVAC3-CC4 (SV312, CC408) are as follows:

- MAXELM = 5, maximum number of elements for which solubility is explicitly calculated in the vault (i.e., U, Pu, Th, Tc, Np);
- MAXIFI = 3, maximum number of final ionic strength indices for vault solubility calculations;
- MAXISI = 3, maximum number of initial ionic strength indices for vault solubility calculations;
- MAXLCH = 10 maximum length of radionuclide decay chain;
- MAXLOC = 10 maximum number of discharge locations to biosphere;
- MAXNOD = 200 maximum number of nodes in geosphere transport network;
- MAXNTS = 3000000 maximum number of time series;
- MAXPER = 100, maximum number of periods;
- MAXSEC = 25 maximum number of vault sectors;
- MAXSEG = 200 maximum number of segments in geosphere transport network;
- MAXSPE = 30, maximum number of species in vault solubility calculations;
- MXBSTA = 4, maximum number of unique biosphere states;
- MXCHEM = 25 maximum number of chemical elements (increased in CC4 from SV311 default value);
- MXCOMP = 20 maximum number of compartments in a multi-compartment group
- MXFOOD = 5 maximum number of food types in biosphere;
- MXGDLN = 3 maximum number of nuclides where the groundwater dilution limit is applied;
- MXGCNQ = 400 maximum number of geosphere consequences stored;
- MXMNRL = 20 maximum number of different minerals important for sorption in each segment;
- MXMTRX = 2 maximum number of matrix materials;
- MXNAME = 200 maximum number of names to dimension model variables;
- MXNHUM = 4 number of non-human biota;
- MXOXST = 2 number of redox states of groundwater in geosphere;
- MXCPCL = 20 maximum number of chemical property classes for segments in geosphere transport network;
- MXFELD = 4, number of field types in the biosphere;
- MXFIRE = 3, number of fire types in the biosphere;
- MXGSTA = 10, maximum number of geosphere states;

- MXPPCL = 20 maximum number of physical property classes for segments in geosphere transport network;
- MXSPEC = 40, maximum number of chemical species (i.e. elements) modelled (increased in CC4 from SV311 default value);
- MXSTSZ = 60000000 maximum storage size for common blocks;
- MXTERR = 7, number of terrestrial biota (MEAT, MILK, BIRD, PLANT, MAMLN, BIRDN, PLNTN);
- MXTSTP = 900, maximum number of time steps in a time series;
- MXWATR = 3, number of types of water sources;
- NANIML = 3 number of terrestrial animal food types used in the biosphere;
- NBMAT = 2, number of building materials;
- NCCOMP = 6, number of biosphere compartments used for chemical toxicity ;
- NCOMP = 18, number of compartments in the biosphere consequences;
- NDEPOS = 3 number of deposition sources;
- NHNANI = 3 number of animals receiving a dose;
- NHTANI = 2 number of terrestrial animals receiving a dose;
- NHTERR = 3 number of terrestrial non-humans biota receiving a dose;
- NPATH = 26 number of possible pathways by which man receives dose;
- NPATHB = 10 number of possible pathways by which birds receive dose;
- NPATHF = 3 number of possible pathways by which fish receive dose;
- NPATHP = 5 number of possible pathways by which plants receive dose;
- NPATHM = 10 number of possible pathways by which mammals receive dose;
- NSOIL = 4, number of types of soil;
- NTERR = 4, number of terrestrial food types;
- NLTIM = 25, number of user-defined times used in outputting a time series to the PAR and OUT files.

3. EXECUTION OF SYVAC3-CC4

This section assumes the existence of a SYVAC3-CC4 executable. See Appendix K for information on creating the executable. For more information on changing the code, see the programmer's guide in Appendix J.

3.1 NORMAL RUN

For a simulation, the user must supply the main input file, certain system model INCLUDE files, and the Solubility, Sorption and Geosphere fixed parameter and network data files. All the possible types of SYVAC3-CC4 input files are listed in Section 5.1 (note that all are not required). Input files may be obtained by modifying existing files, or by use of special input file preparation tools. It is worth noting that the input parameters are provided as probability distribution functions to account for their uncertainty and for possible use in probabilistic simulations (although a constant value is also supported). More information on the parameter distributions supported by SYVAC3 is provided in Andres (1993).

The user must first create a directory in which to execute the simulation. Then the user must copy into this directory the required input files listed in Table 5.1. This includes the SP*.INC, DP*.INC and CQ*.INC files since they are needed by SYVAC3 during execution. Once these files are in place, the simulation can be run in either batch mode using a command file or interactively from the MS-DOS prompt.

In interactive mode, the executable file name is invoked. SYVAC3-CC4 will return with a copyright screen and ask for the 4-letter designation of the input file (which must be in upper case). For example, the input file might be SV01.INP, in which case the input file name entered is SV01. The code will then ask if this is a new run or restart run. The response is either N, n, R or r, depending on the answer.

Appendix A contains an example command file that copies into an existing directory all required files, submits the simulation, renames the output files to an appropriate name, and then deletes the INCLUDE files that are no longer needed from the directory.

3.2 RESTART PROCEDURE

It may be desired to restart and continue a multiple run simulation (generally these are probabilistic runs, but this is not required). In order to restart the simulation, all input files listed in Table 5.1 must be available as well as all output files listed in Table 5.5, except for time series files which are not required for a restart. The simulation is then resubmitted with a "R" or "r" for Restart replacing the "N" or "n" for New in the prompt file (Appendix A).

The original output files will be appended, except for the *.LPT file which is overwritten. Caution should be used when performing a restart and it is advised that a new directory be used with a copy of the output files be used rather than the originals since, if the restart fails, it may damage these files. Generally a restart is only performed when a system model error has caused the simulation to stop or the user wants to extend an existing multiple simulation output file. In the case of a system error, a successful restart cannot be guaranteed but is normally possible.

4. ERROR AND WARNING MESSAGES

Warning and error messages from a model are sent to the screen and to the *.LPT output file. These messages have the following format:

```
--WARNING IN RUN #      nn --      (MODNAM)
informative message of one or more lines
```

```
**ERROR IN RUN #      nn **      (MODNAM)
informative message of one or more lines
```

The messages begin with the string "--WARNING" or "***ERROR" and indicate which run number is affected and which module issued the warning. The module identification may be of primary interest to a programmer, but in some cases makes a message unique or the meaning of a message clearer for a user when more than one module can produce the same message.

Warning messages may indicate unusual conditions or simply provide information to the user. The code continues execution. An example of a warning generated by an unexpected condition is shown below. In this example, the warning (written by the module ASSVAL) indicates that the input parameter LEACHC has a value that is outside of the probability distribution bounds specified in the *.INP main input file.

```
--WARNING IN RUN #      1 --      (ASSVAL)
VALUE      1.000000D-05 IS AT OR OUTSIDE QUANTILE BOUNDS FOR LEACHC
```

In the following example, the warning message is used to simply report the current simulation number so that progress of a set of simulations can be monitored.

```
--WARNING IN RUN #      1 --      (SIMLAT)
BEGINNING SIMULATION
```

Error messages usually indicate unusual conditions of a more serious nature. With errors, the run may either stop the run immediately, complete some additional calculations and then stop, stop this simulation and go on to the next simulation in the run, or attempt to continue operating. If a run is stopped, no further calculations are done and no further results appear in the *.PAR and *.OUT files. The status of each simulation is classed as:

- ACCEPTED if the simulation completed, with all output results calculated.
- REJECTED if the simulation is stopped for problems with calculating dependent parameters. No time dependent simulation is done. In the *.PAR and *.OUT files, not all dependent parameters are evaluated and all consequences have artificial values.
- ONHOLD if the simulation is stopped for problems during the time dependent part of the simulation. The *.PAR and *.OUT files have all dependent parameters, but all consequences have large positive values.

An example of an error message is shown below. In this case, a requested file MDNAA10.Q01 could not be opened by the Fortran module SKIP.

```
**ERROR IN RUN #      1 **      (SKIP  )
FILE MDNAA10.Q01 COULD NOT BE OPENED.
```

Warning and error messages generated by the CC4 model are listed in the following sections. The information about the originating module is appended to end of the actual message to ensure the uniqueness of the message and for potential use by programmers or designers. In the *.LPT file this information appears on the previous line as shown in the examples above.

4.1 WARNING MESSAGES

ANGLE OF DISPOSAL ROOMS TO GEOSPHERE X-AXIS IS LARGER THAN 180 DEG (VLGDEP).

The sampled parameter, RMANGL, is larger than 180. The calculations continue normally.

ATTEMPT TO STORE TOO MANY TIME SERIES. THE LIMIT *MaxNumberOfTimeSeries* CAN BE RAISED BY CHANGING MAXNTS.INC' (STORTS)

The sampled parameter, MAXNTS, is larger than 3000000. The calculations will continue normally but some information may be lost. The user can increase MAXNTS and recompile.

BEGINNING SIMULATION (SIMLAT)

Message for information only. It allows the user to monitor the progress of a run with many simulations.

CALCULATION ORDER DETERMINED, VECTOR SIZE IS *NumberNodes* (NETORD)

Indication that geosphere node calculation order was determined successfully and the number of nodes in the calculation set. The list of nodes in calculation order is given in the DOS file.

DISCHARGE LOCATION INDEX FOR *FRAC3DVSSliceLabel* TOO SMALL OR TOO LARGE FOR NETWORK, DATA NOT USED (GETF3D).

The discharge location index used in the FRAC3DVS control input file is either less than 1 or greater than NBLOC and therefore invalid so the FRAC3DVS data is ignored.

DISCHARGE LOCATION TYPE *LocationType* HAS NO SEDIMENT LAYER (GEODEP).

A sediment layer is normally expected for an aquatic discharge, type AQUA, or a wetland discharge, type BOG, but none has been found.

DISCHARGE LOCATION TYPE *LocationType* SHOULD NOT HAVE A SEDIMENT LAYER (GEODEP).

Sediment should occur only under aquatic discharges such as lakes and streams (AQUA) or wetlands (BOG). This warning occurs if a sediment layer is found associated with another discharge type such as terrestrial (TERR) or gaseous (GAS).

FRAC3DVS CONTROL FILE FOUND FOR THIS SIMULATION (GETF3D).

Message for information only. This message tells the user that the FRAC3DVS data will be used in this simulation. If the user does not want FRAC3DVS data to be used, then the F3D*.FXD file must be removed from the set of input files required for the simulation.

FRAC3DVS DATA FOR SPECIES *NuclideName* EXPECTED IN DATA FILE *FileName* (GETF3D).

Message for information only. This message tells the user that the FRAC3DVS data for a particular nuclide is expected in a certain file.

FRAC3DVS DATA USED, - FURTHER USE IGNORED (GETF3D).

The FRAC3DVS data was read and used for the first simulation in this case, other simulations will use CC4 data.

GEONET DISCHARGE LOCATION *LocationType* ASSOCIATED WITH FRAC3DVS
FRAC3DVSSliceLabel (GETF3D).

Message for information only. This message tells the user which discharge location number is associated with each the FRAC3DVS slice label.

GW VELOCITIES ARE INPUT WITH A WELL PRESENT. WELL OPERATION BASED ON VELOCITY IN SEGMENT *wellSegment* AND THE TRANSPORT CALCULATIONS WILL BE INCONSISTENT. (ADDWEL)

Warning to user that geosphere transport calculations and the well operations of capture fraction, surface water flow, etc. cannot be done consistently under these conditions.

INCREASE MAXLOC BY 1 FOR FIELD WITHOUT DISCHARGE FOR BIOSPHERE
GLACIATION STATE *StateNumber* (FLDARE).

Increase the value of MAXLOC in MAXLOC.INC by at least one and recompile the source code to accommodate an extra field without a discharge.

INSUFFICIENT ROOM TO STORE FRAC3DVS DATA, REMAINDER IGNORED (REAF3D).

There is more FRAC3DVS data then can be stored in the arrays to generate the time series. Either reduce the data or increase the array size parameter, MXF3DT, and re-compile and re-link.

INSUFFICIENT ROOM TO STORE NEXT CONSEQUENCE PREVIOUS RESULT *Label*
DROPPED AND WRITTEN HERE: *TimeOfMaxFlow* *MaxFlow* *IntegratedFlow* (GNETCQ).

More geosphere consequences are requested in the NET**.FXD input file than space allocated in the model code. The consequences dropped will not be available in the PAR or OUT files but will written to the LPT file. Reduce the number of consequences requested in the geosphere NET**.FXD file or the number of nuclides in the chains list in the main input file. The product of the number of nuclides and the number of consequence node locations must be less than MXGCNQ (=400).

INVALID CALL TYPE *CallFlag* SHOULD BE "MIN" OR "MAX". MXMNVC SET TO FIRST ELEMENT OF VECTOR (MXMNVC).

"MIN" OR "MAX" was not used in the call to MXMNVC. The first element of the vector is returned.

KD FOR SEGMENT= *SegmentNumber* MINERAL= *MineralNumber* ELEMENT= *Element*
WAS NEGATIVE *KDValue* AND HAS BEEN SET TO ZERO (RETDEP).

The KD is a ratio of concentrations and its value cannot be less than zero. The value is determined from the data in the SORxx.FXD file and the data should be checked for errors. The negative value calculated has been reset to zero (no sorption) and the simulation continued.

MATRIX MAT. IS NOT URANIUM, RADIOLYSIS DISSOLUTION REQUESTED BUT CANNOT BE USED (FULRAD).

The matrix material is not uranium so the radiolysis dissolution cannot be used but was requested by the user. The user must change the matrix degradation type to avoid this message.

NETORD RETURNED FAILED (GETNET)

Indication that geosphere node calculation order was not determined successfully. An error message follows.

NETORD RETURNED SUCCESSFUL (GETNET)

Indication that geosphere node calculation order was determined successfully from the node connectivity defined in the NET**.FXD file.

NEXIDX greater than MAXNOD while final packing (NETORD)

A problem occurred during the determination of the geosphere network calculation order. An error message follows. The user should not normally see this message. Contact the code administrator.

NO OF COMPARTMENTS FOR MULTIC RESPONSE FUNCTIONS ADJUSTED TO BE IN ALLOWED RANGE NEW VALUE = *NewNumberOfCompartments* (STADEP).

The number of compartments specified in the input file as DCMPT must be less than or equal to the maximum number of compartments MXCOMP-2 since two extra compartments are required for a boundary compartment and for a sink compartment. The code will reset the number of compartments to be used to the upper limit of MXCOMP-2.

NO ROOM TO STORE TIME SERIES. EARLIER TIME SERIES WILL BE OVERWRITTEN. THE LIMIT OF *Number* TIMES CAN BE RAISED BY CHANGING MXSTSZ (STORT2).

The time series storage limits have been reached and the storage space is being reused. Time series created earlier in the simulation are overwritten. This is a normal condition, but in a long and complex simulation, may lead to the error "TIME SERIES ... HAS BEEN OVERWRITTEN..."

NO NUCLIDE DATA FOUND IN CONTROL FILE (GETF3D).

There is no nuclide data in the FRAC3DVS control input file so no FRAC3DVS data is used.

NO VALID DISCHARGE DATA FOUND IN CONTROL FILE (GETF3D).

There is no discharge location data in the FRAC3DVS control file so the FRAC3DVS data is ignored.

NO WELL FOUND IN THIS NETWORK (ADDWEL).

Message for information only. Wells are commonly occurring discharges of groundwater from a geosphere. However, a well discharge is not required.

PARAMETER *ParameterName* IS IN COMMON BLOCK *CommonBlockName* BUT NOT IN THE INPUT FILE (CHECKI).

The indicated parameter is in a submodel common block, but not found in the input file. The list of SP, DP, and CQ INCLUDE files in the input file is inconsistent with the lists of parameters in the sampling methods.

PECLET NUMBER *Number* IN SEGMENT *SegmentNumber* TOO SMALL FOR MATRIX DIFFUSION (MATDEP).

The Peclet number is less than 1 so no matrix diffusion effects are applied.

POROSITY DUE TO MICROFRACTURES HAS A VALUE OF *PorosityValue* WHICH IS OUTSIDE THE ALLOWABLE RANGE OF 0 TO 1. SIMULATION TERMINATED (MATDEP). Non-physical value of porosity. The fracture porosity is determined from the ratio SGFAPT/SGFSPA. Check the values of sampled parameters SGFAPT and SGFSPA.

POROSITY OF MATRIX HAS A VALUE OF *Value* WHICH IS OUTSIDE THE ALLOWABLE RANGE OF 0 TO 1. SIMULATION TERMINATED (MATDEP). Non-physical value of porosity. Check the values of the sampled parameters SGPROS, SGFAPT, and SGFSPA.

RESPONSE AREAS FOR *Nuclide* VAULT SECTOR *SectorNumber* ARE *Value* +OR- *ErrorValue* VS SYVAC *Value* +OR- *ErrorValue* - (SIMTRA).

The indicated response function time series for transport through the vault is outside the results of a bounding test performed by SYVAC3 (based on the area under the time series). If this warning occurs, it generally requires no action, although the user should check the relative values to see if the discrepancy is large enough to be a concern to them. The simulation could be rerun with a smaller time series target fractional error and/or a larger allowed number of time points to see if the warning is eliminated.

SIMULATION TIME *TLIMIT* EXCEEDS MAX TIME OF FRAC3DVS OUTPUT *FRAC3DVSTLIMIT* (SIMF3D).

The simulation time is greater than the last time present in the FRAV3DVS output. The last data value in the FRAC3DVS output will be used to fill in the values for the remaining times up to *TLIMIT*.

SEDIMENT THICKNESS IS .LT. 0 FOR DISCHARGE LOCATION *LocationNumber* OF TYPE *LocationType* (ADDOSS).

The sediment thickness is negative. This is physically meaningless. There is an error in the input data. The sediment thickness is reset to zero and execution continues.

SEGMENT *SegmentNumber* HAS A NEGATIVE GROUNDWATER VELOCITY OF *VelocityValue* (GWVDEP).

The message is for information. Geosphere transport segments are usually defined to follow the groundwater flow field such that all groundwater velocities are positive. The indicated segment has a negative velocity. The treatment of dispersive transport is different in the model when the groundwater flow is countercurrent to the direction of transport.

SELECTED PARAMETER *Parsnm* IS IN THE FILE, BUT NOT IN THE MODEL COMMON BLOCKS (RINDEX)

The parameter is in input file, but not in the submodel common blocks. Check if proper include file(s) were used to run the simulation.

SORPTION DATA FOR ELEMENT *Element* FOUND WHEN DATA FOR ELEMENT *Element* WAS EXPECTED IN FILE *SorptionDataFile* (GETSOR).

Sorption data is out of order or missing in geosphere sorption fixed data file. The data must have the same order of elements as the order of elements in the main input file in parameter INVPKG. Check for use of the wrong sorption data input file, reorder the input file or regenerate the sorption data file for this nuclide group using the input file generation tools.

SPECIES *NuclideName* NOT FOUND IN THIS GROUP, DATA NOT USED (GETF3D).

The nuclide name specified in the FRAC3DVS control file is not present in the nuclide group currently being simulated so the data for that nuclide is ignored.

STABLE NUCLIDE *NuclideName* FOUND, FRAC3DVS DATA NOT USED (SIMF3D).

A stable nuclide was found in the list of nuclides so the FRAC3DVS data will not be used and the data for that nuclide will be ignored.

TIME SCALE FOR CONSTANT CORROSION DISSOLUTION OF WASTEFORM <= ZEREQU (SMCSCR).

The time for constant corrosion dissolution of wasteform, TMDSSL, is too small. The check on this value avoids a possible divide by zero error.

TIME SERIES *TimeSeriesNumber* HAS BEEN OVERWRITTEN, AND CANNOT BE RETRIEVED. SO FAR, *Number* TIME SERIES HAVE BEEN STORED, USING *Number* TIME STORAGE LOCATIONS. (RETTS)

The calculations continue normally. Earlier, less used time series will be overwritten. To ensure the time series remains accessible it should be accessed, put on the time series stack (RETTS) or the time series refreshed.

UNIDENTIFIED DEGRADATION TYPE = *DegradationNumber* (SIMWFM, DKFST).

An invalid degradation type was entered for a matrix material. Valid degradation numbers are 1 through 4.

VALUE *Number* IS AT OR OUTSIDE QUANTILE BOUNDS FOR *ParameterName* (ASSVAL).

A value is being assigned to a sampled parameter using the ON FILE method but the value is outside the range that would be assigned by the RANDOM and QUANTILE methods. The value requested is assigned and overrides the range indicated in the input file.

VECTOR HAS ZERO LENGTH (MXMNVC).

The vector passed into this function has a length of zero. The first element in the vector is returned, whatever it happens to be at the time.

WORKING VECTOR PACK COUNT *MaxCount* EXCEEDED (NETORD)

The working vector used in determination of geosphere node calculation order has been filled and packed more than the allowed number of times. There is likely a problem with the net connectivity tables in the NET**.FXD file. An error message follows.

WORKING VECTOR PACKED TO *NewSize* FROM *OldSize* (NETORD)

The working vector has been filled during the determination of the geosphere node calculation order and has been packed to create more room.

WELL DEMAND = *Value* > *MaximumWellDemand*. SOURCE FRACTIONS AND MODIFIED AREAS WILL BE EXTRAPOLATED AND MAY BE UNREALISTIC (SSPWEL).

For the CC4 site specific well model as applied in the third case study and the horizontal borehole study, the maximum well demand is limited. This model and site specific module must be revised for each application. Check that the correct site specific well model is applied.

WELL EXISTS WITH NO SEGMENT BYPASSING IT FROM WELL CAPTURE NODE *NodeNumber* (WELDEP).

When there is a well in the geosphere model as a discharge point for groundwater, an alternative flow path must also be present that leads any contaminants not captured by the well to discharge somewhere else. This network has a well but no well bypass pathway has been found. The network data in the NETxx.FXD file must be corrected.

ZERO DENOMINATOR IN RESPONSE *Nuclide* VAULT SECTOR *SectorNumber* (SIMTRA).
A divide by zero was prevented in the calculation of a boundary integral response function in the buffer, backfill or EDZ for the specified nuclide and vault sector. The divide by zero operation is bypassed and execution continues. The results may be unreliable for this nuclide. The input parameters and intermediate results should be checked for unreasonable or inconsistent values.

4.2 ERROR MESSAGES

BAD CALCULATION ORDER (GETNET)

The geosphere node calculation order was not determined successfully. There is a problem with the node connectivity defined in the NET**.FXD file. The run is stopped.

CALCULATION NODE *NodeNumber* NOT FOUND AS AN OUTLET NODE (SIMGEO).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The segment and node connectivities or the list of calculation nodes are incorrect. Correct the segment and node information in the network file.

CANNOT OPEN FILE *OutputFiles* (INTRO)

The output files already exist and will not be overwritten. Either remove them, move them, or rename them. The run is stopped.

CAN NOT USE RMSTFR WHEN THERE IS NO NEXT SEGMENT FOR SEGMENT *SegmentNumber* (SIMGEO).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The mass transfer response function can only be used when there is a segment following the segment in the network that is using RMSTFR. Correct the information in the network file.

CASE CONTROL INFORMATION NOT ALL FOUND, CHECK THE INPUT FILE *InputFile* (INTRO).

The case control information near the front of the input file is not correct. Check for correct spacing and record continuation characters for each logical record.

COMMON BLOCK *CommonBlockName* WAS NOT FOUND (RETCMN, STOCMN)

A SP, DP, or CQ common block is missing from simulation area. The run is stopped. Ensure the required common block is available to the simulation area, remove any output files created and resubmit the simulation.

COULD NOT OPEN FRAC3DVS DATA FILE *FileName* (REAF3D).

A FRAC3DVS data input file could not be opened. Check file permissions and check if the file exists in the run directory.

COULD NOT READ FRAC3DVS DATA FILE *FileName* (REAF3D).

A FRAC3DVS data input file could not be read. Check the format of the data file.

DATA NOT SUCCESSFULLY READ FROM FILE NET**.FXD (NETDEP).

The geosphere network data file (NET**.FXD) was opened successfully but the data set was not as expected. The run is stopped. Check the format and content of the data in the NET**.FXD file.

DATA NOT SUCCESSFULLY READ FROM FILE SOL**.FXD (SOLDEP).

The solubility data file (SOL**.FXD) was opened successfully but the data set was not as expected. The run is stopped. Check the format and content of the data in the SOL**.FXD file.

DATA NOT SUCCESSFULLY READ FROM FILE SOR**.FXD (GEODEP).

The sorption data file (SOR**.FXD) was opened successfully but the data set was not as expected. The run is stopped. Check the format and content of the data in the SOR**.FXD file.

DAUGHTER RN222 IS BEING USED WITHOUT PARENT RA226 (SIMATT).

If radionuclide RN222 is simulated, then its parent RA226 must also be simulated in order to determine transport of terrestrial contributions to the atmosphere for RN222. The run is stopped. Correct the list of radionuclide chains being simulated.

DISCHARGE NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDOSS).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A node indicated to be a discharge node to the biosphere was not found as an outlet node for a segment. Correct the segment and node information in the geosphere network NET*.FXD file.

FAILED READING FIXED NETWORK DATA (GETNET)

Failed reading data from fixed geosphere network file. Check the format of the network file.

FIRST NUCLIDE IN CHAIN *NuclideName* CANNOT BE IN SECULAR EQUILIBRIUM WITH PREVIOUS NUCLIDE (CHAINS).

Check that the first nuclide in a chain does not have an "=" indicating secular equilibrium.

FRAC3DVS RUNID/FILEID TOO LONG - *FileName* (GETF3D).

The FRAC3DVS data input file name is too long once the run identifier and file identifier are concatenated together. Shorten either or both identifiers.

FRAC3DVS UNIQUE FILE NAME TOO LONG *FileName* (GETF3D).

The FRAC3DVS data input file identifier is too long. Shorten the identifier.

FUEL DOSE VALUES CANNOT BE INTERPOLATED BECAUSE TIMES MAY NOT BE MONOTONIC (ALPHDS, BETADS, and GAMADS).

An appropriate interpolation interval cannot be found to calculate the dose at a particular time. The run is stopped. Check that the times in the input parameter lists ALPHTI or BETATI or GAMATI are in increasing order, start at times less than the start of the simulation, and end at or after the end time of the simulation.

FUEL DOSE VALUES OUTSIDE ARRAY BOUNDS (ALPHDS, BETADS, GAMADS).

The number of requested entries in the fuel radiolysis dose rate time series is larger than the allowed array storage. The run is stopped. The value of input parameter NOALPHA or NOBETA or NOGAMMA is too large.

HALF LIFE *Value* OF NUCLIDE *NuclideName* IS TOO SMALL (DEPPAR).

The half-life of a nuclide is shorter than the allowed value of MNHLIF years. The run is stopped. Correct the input value for HLIFE or change the nuclide chains list to delete this nuclide (it's effect should be considered within the dose coefficient of its parent).

INPUT OF DISTRIBUTIONS STOPPING BECAUSE OF ERROR IN INPUT (CHECKI)

Usually caused due to problems with correlated parameters or problems with ranges of the parameter distributions in the main input file.

INVALID DISCHARGE TYPE *DischargeType* FOR DISCHARGE *DischargeLocation* (NETDEP).

The discharge type is invalid. It must be anyone of 1 thru 5 or 9 for any discharge location.

INVALID GROUNDWATER VELOCITY FUNCTION INDICATOR (ADDOSS, ADDWEL, GWVDEP).

There is an error in the geosphere network NET**.FXD file. The run is stopped. Groundwater velocity function indicator found in the network file is not supported. Valid values are 1, 2, 3, 4, 5, or 6. Correct the information in the network file.

INVALID IRRIGATION TYPE *IrrigationType* FOR FIELD *FieldType* STATE *StateNumber* (SOILIR).

The irrigation type is not "WELL", "LAKE", or "NONE". The run is stopped. Correct the values for parameters that control irrigation.

INVALID PROVISIONAL DOMESTIC WATER SOURCE, PRODOM: *WaterSource* (DWASRC).

The domestic water source, defined by sampled parameter PRODM, is not defined as "WELL" or "LAKE". The run is stopped. Correct the values for PRODM. Acceptable values are either 1 or 2.

INVALID SOIL TYPE *Number* (WTRSRC)

INVALID SOIL TYPE; SHOULD BE NO GREATER THAN *Number* (WTRSRC).

The soil type index is greater than the number of soil types available or less than 0. The simulation is placed stopped. Correct the value of sampled parameter DPSTYP. Valid values are 1, 2, 3, or 4.

INVALID TIME SERIES INDEX (VALUE = *Number*) (RETTS)

Attempt to use a time series not yet created. Not usually seen by the user. May be caused by unexpected data for the model or by programming problem. Usually causes simulation to be stopped.

INVALID VALUE OF PROIRR(VEGPCH): *Number* (FWASRC).

Source of water for irrigating the vegetable patch is set to an invalid value. It should be 0 or 1. The run is stopped. Check value for input parameter PROIRD.

INVALID VALUE OF PROIRR(FORAGE): *Number* (FWASRC).

Source of water for irrigating the forage field is set to an invalid value. It should be 0 or 1. The run is stopped. Check value for input parameter PROIRD.

INVALID VAULT RELEASE TYPE *ReleaseType* FOR VAULT SECTOR *SectorNumber* (NETDEP).

The vault release type is invalid. It must be 1 or 2.

INVALID VAULT SECTOR NUMBER *SectorNumber* AT POSITION *Number* (SIMGEO).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A vault sector number assigned to a geosphere source node is equal to zero. Correct the information in the network file.

LAST RUN REQUESTED ALREADY FINISHED. NO PROCESSING DONE FOR THIS CASE (INTRO).

When using multiple ranges for simulation numbers, run will not be rerun if it is already completed. The simulation will not be run. Check requested run ranges in the main input file; they should not overlap.

MORE THAN ONE WELL IN NETWORK NOT ALLOWED (ADDWEL)

Check that there is only one well in the list of discharge locations specified geosphere network file.

NET**.FXD COULD NOT BE OPENED (GETNET).

The geosphere network datafile (NET**.FXD) could not be opened. The run is stopped. Check the name, location, and protection of the network file.

NETWORK MAY BE CIRCULAR, NO CALCULATION ORDER CAN BE DETERMINED (NETORD)

There is likely a problem with the net connectivity tables in the NET**.FXD file. The run is stopped.

NO RESPONSE FUNCTION NO. *Number* (SIMGEO).

There is an error in the geosphere network NET**.FXD file. The run is stopped. Response function indicator found in the network file is not supported. Valid values are 1, 2, 3, 4, 5 or 6. Correct the information in the network file.

NO SEGMENT FOUND WITH OUTLET NODE *NodeNumber* (FRFFOB).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A node in the network leading back from a discharge node to the biosphere of type AQUA, TERR, or BOG was not found as an outlet node for a segment. Correct the segment and node information in the network file.

NO TIMES IN THE TALBOT INTERVAL (RESPCY).

No result for an attempted calculation of an inverse Laplace transform. The user should not see this message. It indicates a programming error. The run is stopped. Consult the code owner.

NODE *NodeNumber* NOT FOUND AS DISCHARGE NODE OR AS INLET TO ANOTHER SEGMENT. CANNOT FIND DISCHARGE LOCATION FOR WELL BYPASS TO MODIFY FOR WELL FLOWS (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The segment and node connectivities near to the well nodes are incorrect. When there is a well in the geosphere model as a discharge point for groundwater, an alternate flow path must also be present that leads the contaminants not captured by the well past the well to discharge somewhere else. This network has a well but the well bypass pathway could not be followed to another discharge location. Correct the segment and node information in the network file.

NUCLIDE *NuclideName* WAS NOT FOUND IN THE INVENTORY. CHECK THAT THE PARAMETER LONG NAMES FOR THE INVENTORY HAVE THE FOLLOWING FORMAT: "INVENTORY, V " (CHAINS).

One parameter in the input file must have the long name "INVENTORY, V " in order to create the cross reference lists for chain order and parameter order of the nuclides. Check the main input file for this long name.

NUCLIDE NOT FOUND SHOULD BE I-129, C-14, OR CL-36 (GLOWT1, GWDLTN).

This calculation applies to only these six nuclides, but an attempt has been made to use it for a different nuclide. The user should not see this message. It indicates a programming error. The run is stopped. Consult the code owner.

NUCLIDES *FirstNuclide* AND *CurrentNuclide* CANNOT BE IN SECULAR EQUILIBRIUM (DEPPAR).

The *CurrentNuclide* cannot be in secular equilibrium with the *FirstNuclide* because the *Current Nuclide* has the longer half-life. The run is stopped. Correct the chains list or correct the values for HLIFE in the main *.INP input file.

OVERBURDEN NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDOSS).

There is an error in the geosphere network NET**.FXD file. The run is stopped. An overburden node is a node adjacent in the network to a sediment node and it was not found in turn as an outlet node for a segment. Correct the segment and node information in the network file.

PARAMETER *ParameterName* IS OUTSIDE THE 1 TO *ParameterRange* INCLUSIVE RANGE (STADEP)

The cross reference parameters GIXDS or BIDXs are not in their value ranges.

The simulation is REJECTED. The values for the indicated parameter should be corrected.

PARAMETER *ParameterName*, *ParameterValue* THIS IS OUTSIDE THE *ParameterRange* REQUIRED FOR THE BIOSPHERE (PREBIO, PREDOS).

There are many potential error messages from the biosphere of this form that report a violation of a check on preconditions for the biosphere transport model and the biosphere dose model. The simulation is REJECTED. The values for the indicated parameter should be corrected.

PROGRAM STOPPING FOR ABOVE ERRORS (DEPPAR).

The run is stopped. Previous error messages indicate the reasons.

READING MATRIX MATERIALS (MATRXM).

Message for information only unless the program stops after reading an incorrect matrix material at the end of the main input file.

REFERENCE WELL NODES INCONSISTENT WITH WELL DEPTH (ADDWEL).

There is an error in the data. The run is stopped. There may be incorrect well reference nodes in the geosphere network NET**.FXD file or the depth of well, sampled parameter DPTHWL, is incorrect. Correct the node information in the network file or the values for DPTHWL. The lower well reference node must lie at lower elevation than the well aquifer node, which is the node in the network adjacent to the node designated as the well discharge node.

ROOT OF GROUNDWATER DIVIDE FUNCTION NOT FOUND (GWDIV).

The solution to the groundwater divide equation was not found. The simulation is REJECTED.

SAMPLING METHOD *Method* IS INVALID. IT MUST BE 'RANDOM' OR 'RANDOM 2' OR 'QUANTILE' OR 'ON FILE' (ASSVAL)

The only allowed sampling methods that can be used to assign values to the sampled parameters are those listed. Correct the erroneous sampling method in the input file.

SEARCH FOR WELL BYPASS DISCHARGE HAS LED TO THE WELL DISCHARGE (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The segment and node connectivities near to the well nodes are incorrect. When there is a well in the geosphere model as a discharge point for groundwater, an alternate flow path must also be present that leads the contaminants not captured by the well past the well to discharge somewhere else. This network has a well but following the well bypass pathway has led back to the well discharge again rather than to an alternate discharge location. Correct the segment and node information in the network file.

SEDIMENT NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDOSS).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A node adjacent in the network to a discharge node to the biosphere (a sediment node) was not found in turn as an outlet node for a segment. Correct the segment and node information in the network file.

SELECTED PARAMETER *ParameterName* IS IN THE FILE, BUT NOT IN THE MODEL COMMON BLOCKS (RINDEX).

The indicated parameter is in the input file, but not found in a submodel common block. The run is stopped. The list of SP, DP, and CQ *.INC files in the input file is inconsistent with the lists of parameters in the sampling methods.

SGPERM (*SegmentNumber*) = *Value* SUPPLY PERMEABILITY FOR SEG = *SegmentNumber* (GEODEP).

A valid value for the permeability for the listed segment is required, but an invalid value of less than 1.0E-30 was found. The simulation is REJECTED. Supply or correct the value for sampled parameter SGPERM for the indicated segment.

SIMULATION ERROR (occurs in many modules in biosphere model).

An error in a calculation or time series operation has occurred. The simulation is stopped. Previous error messages should be present that describe the error condition.

SOL **.FXD COULD NOT BE OPENED (GETSOL).

The solubility datafile (SOL **.FXD) could not be opened. The run is stopped. Check the name, location, and protection of the input solubility file.

SOR **.FXD COULD NOT BE OPENED (GETSOR).

The sorption datafile (SOR **.FXD) could not be opened. The run is stopped. Check the name, location, and protection of the input sorption file.

SPECIAL UO₂(CO₃)₃₋₄ SPECIES NOT FOUND (SOLCRR).

There is a problem with the Uranium species list used for calculating Uranium solubilities. The specified Uranium carbonate species must be present in the solubility calculation. Correct the data in the files for MNUM and the Pn variables. The user will not normally see this error

message unless an inconsistent/incorrect revision is made to the solubility calculation and/or database.

STABLE NUCLIDE *NuclideName* IS NOT AT THE END OF A CHAIN (DEPPAR).

A nuclide has a half life greater than the maximum allowed value of MXHLIF (1.0E+30 years) indicating it is a stable nuclide and it is not found at the end of a decay chain. This condition is invalid; a stable nuclide can have no further progeny. The run is stopped. Correct the chains list or correct the values for HLIFE in the main *.INP input file.

SUM OF LOSS RATES IS LESS THAN OR EQUAL TO ZERO (RSPNLW).

The total loss rate from the lake water must be greater than zero, but an invalid value was found. The run is stopped. The loss rate is calculated from

$\text{SEDSOR(NUC)} + (\text{AREATE} * \text{RUNOFF}) / (\text{AREAAQ} * \text{LD}) + \text{DECAY(NUC)} + \text{DEGASL(NUC)}$.
Check values for related sampled parameters.

SUPPLY AQUIFER HYDRAULIC CONDUCTIVITY IN "SGHYCO" FOR SEGMENT *SegmentNumber* (ADDWEL).

A valid value for the hydraulic conductivity for the listed segment is required, but an invalid value of less than 1.0E-30 was found. The run is stopped. Supply or correct the value for sampled parameter SGHYCO for the indicated segment.

SUPPLY AQUIFER POROSITY IN "SGPROS" FOR PROPERTY CLASS *PropertyClass* (ADDWEL).

A valid value for the porosity for the listed segment is required, but an invalid value of less than 1.0E-30 was found. The run is stopped. Supply or correct the value for sampled parameter SGPROS for the indicated segment.

SUPPLY NON-ZERO TRANSFER LENGTH IN SGTFRL FOR SEGMENT *SegmentNumber* (SIMGEO).

When using the mass transfer response function a valid value for the transfer length for the segment must be supplied but an invalid value of less than 1.0E-30 was found. The run is stopped. Supply or correct the value for sampled parameter SGTFRL for the indicated segment.

TEMPERATURE TOO SMALL FOR DIFFUSION COEFFICIENT ADJUSTMENT (DIFFUS).

The temperature being used in this function is less than MINPOS. Check temperatures used in the main input file.

TEMPERATURE TOO SMALL FOR VISCOSITY DETERMINATION (VISCOS)

If temperature is less or equal to 0°K, the warning is issued and the value of water viscosity, VISCOS, is assigned a zero. The program will crash if it uses a ground water velocity indicator, GWVFID = 5 or 6 as it will result in division by 0 in the equation for calculation of hydraulic conductivity for segment (ADDWEL, GWVDEP). Also DIFFUS will equal 0, which will lead to "divide by 0" error in MATDEP, RESPCY and HOLCON.

THE NUMBER OF FLOWS IN = *Number* FOR *Compartment* (ACCMSS).

The number of flows into the compartment is less than or equal to 0. Check the number of flows for the compartment. It indicates a programming error.

THE NUMBER OF FLOWS OUT = *Number* FOR *Compartment* (ACCMSS).

The number of flows out of the compartment is less than or equal to 0. Check the number of flows for the compartment. It indicates a programming error.

THERE ARE NO CONTAINERS IN THE VAULT - SEE NCONSC (VLTDEP).

The total number of containers in the vault is zero so further simulation is pointless. The run is stopped. The number of containers is the sum of the values for NCONSC over all the vault sectors. Correct the values for parameter NCONSC.

'THERE ARE NO DISCHARGE LOCATIONS IN AN AQUATIC BODY, AT LEAST ONE IS NEEDED' (PREBIO).

Check that there is at least one aquatic discharge location specified in the geosphere network file.

'THERE ARE NO DISCHARGE LOCATIONS IN A TERRESTRIAL BODY, AT LEAST ONE IS NEEDED' (PREBIO).

Check that there is at least one terrestrial discharge location specified in the geosphere network file.

'THERE IS MORE THAN ONE WELL IN THE MODEL' (PREBIO).

Check that there is only one well in the list of discharge locations specified geosphere network file.

THIS RUN PUT ON HOLD (SIMLAT).

During execution of the time dependent part of the simulation an error has occurred. Check previous error messages for possible reasons for this condition. The simulation is stopped. The consequences will be set to the artificial values assigned in the input file.

TIME LIMIT *Value* FOR SIMULATION OUT OF ALLOWED BOUNDS IN VAULT (DEPPAR).

The end time of the simulation is outside the allowed time limit of 1.0E+08 years for the vault model. The run is stopped. Check the fixed times listed in *.INP main input file, to make sure that they are all greater than zero and less than or equal to 1.0E+08 years.

TIME SERIES *Number* HAS BEEN OVERWRITTEN, AND CANNOT BE RETRIEVED. SO FAR, *Number* TIME SERIES HAVE BEEN STORED, USING *Number* TIME STORAGE LOCATIONS. (RETTS)

Error caused by reuse of time series storage in a long and complex simulation. The warning message "NO ROOM TO STORE TIME SERIES...." should have appeared earlier. Error may be eliminated by reducing the maximum number of times requested for any time series, reducing the complexity of the simulation, or having the program owner increase the amount of time series storage available. Usually causes simulation to be stopped.

TOO FEW TIME SERIES *Number* IN STACK; 2 ARE NEEDED (GLOWT1).

The user should not see this message. It indicates a programming error. The run is stopped. Consult the code owner.

TOO MANY ELEMENTS *Number* IN INVENTORY LIST. LAST ELEMENT IS *ElementName* (CHAINS).

The number of chemical elements in the inventory list is greater than MXCHEM. Reduce the number of chemical elements or increase MXCHEM, re-compile, and re-link.

TOO MANY MATRIX MATERIALS *Number* IN INVENTORY LIST. LAST MATRIX IS *MatrixName* (CHAINS).

The number of matrix materials in the inventory list is greater than MXMTRX. Reduce the number of matrix materials or increase MXMTRX, re-compile, and re-link.

TOO MANY NUCLIDES *Number* IN CHAIN. LAST NUCLIDE IS *NuclideName* (CHAINS).

The number of nuclides in the chain is greater than MAXLCH. Reduce the number of nuclides or increase MAXLCH, re-compile, and re-link.

TOO MANY NUCLIDES *Number* IN INPUT. LAST NUCLIDE IS *NuclideName* (CHAINS).

The number of nuclides in the input is greater than MXSPEC. Reduce the number of nuclides or increase MXSPEC, re-compile, and re-link.

TOO MANY NUCLIDES *Number* IN INVENTORY LIST. LAST NUCLIDE IS *NuclideName* (CHAINS).

The number of nuclides in the inventory list is greater than MXSPEC. Reduce the number of nuclides or increase MXSPEC, re-compile, and re-link..

TOPHAT FUNCTION FAILURE WITH TIMES *LowTime*, *HighTime* AND HEIGHT *Value* (THATTS).

The user should not see this message. It indicates a programming error. The simulation is stopped. Consult the code owner.

TRUNCATED NUCLIDE NAME *NuclideName* THAT WAS TOO LONG (CHAINS).

The number of characters in a nuclide name is longer than the maximum length MXNIDL.

UNIDENTIFIABLE CALL TYPE CALTYP SHOULD BE "TIMES" OR "VALUES" (may be reported from many modules).

The user should not see this message. It indicates a programming error. The run is stopped. Consult the code owner.

UNIDENTIFIABLE VAULT RELEASE TYPE *ReleaseType* AT POSITION *Number* (SIMGEO).

There is an error in the geosphere network NET**.FXD file. The run is stopped. Release type from the vault to the geosphere must be GAS or AQUA. Correct the information in the network file.

UNIT NUMBER OUT OF RANGE (OPENFL).

The FORTRAN file unit number is out of range. It indicates a programming error. The run is stopped. Consult the code owner.

VALUE OF DECAYF *Value* IS TOO SMALL (LEAFCN, LEAFDS, NHEXDS, NHINDS).

The removal rate from plants is too small. The run is stopped. Check the values of parameter XPHLIF.

WELL AQUIFER NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A node adjacent in the network to the well discharge node to the biosphere (the well aquifer node) was not found in turn as an outlet node for a segment. Correct the segment and node information in the network file.

WELL COLLECTION NODE *NodeNumber* NOT FOUND AS OUTLET NODE OF A SEGMENT (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The segment and node connectivities near to the well nodes are incorrect. Correct the segment and node information in the network file.

WELL DEMAND GREATER THAN WELL CAPACITY (WELDEP).

The well demand requested by the biosphere model exceeds the maximum allowed by the geosphere model. The simulation is REJECTED.

WELL DISCHARGE NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. A node indicated to be the well discharge node to the biosphere was not found as an outlet node for a segment. Correct the segment and node information in the network file.

WELL DRAWDOWN NODE NOT FOUND AS SEGMENT OUTLET NODE (ADDWEL).

There is an error in the geosphere network NET**.FXD file. The run is stopped. The segment and node connectivities near to the well nodes are incorrect. Correct the segment and node information in the network file.

WELL TOO CLOSE TO LOWER REFERENCE NODE OR DRAWDOWN NODES MISSING (ADDWEL).

There is an error in the data. The run is stopped. There may be no drawdown nodes in the geosphere network NET**.FXD file or the distance between the well and the drawdown nodes, sampled parameters DISTD1 and DISTD2, is too large. Correct the segment and node information in the network file or the values for DISTD1 and DISTD2.

WRONG INDEX FOR FSCYL FOR NESTED CYLINDERS (FSCYL).

The user should not see this message. It indicates a programming error. The run is stopped. Consult the code owner.

ZERO DENOMINATOR (SOLCY1, SOLCYL).

Zero denominator calculated during attempted solution of set of linear equations that arise in the transport across the buffer, backfill and EDZ. The run continues with the solution set to zero. The results may be unreliable.

5. SYVAC3-CC4 INPUT AND OUTPUT FILES

The SYVAC3-CC4 model, requires the main SYVAC3 ".INP" file, the vault solubility file "SOLnn.FXD", the geosphere network file "NETnn.FXD", and the geosphere sorption file "SORnn.FXD".

Optional files may be used such as the sample files referred to as QUANTILE or ON-FILE files. For example, the "Median Value" simulation uses a quantile file with the quantile value set equal to "0.50". Sample files provide values for sampled parameters in QUANTILE and ON FILE sampling methods. QUANTILE sample files must provide numbers between zero and one. ON-FILE sample files may contain any set of appropriate parameter values. In both cases, all the values needed for a single simulation must appear in a single logical record. There must be as many records as simulations. These files are read as Standard ASCII Files, and so comments and continuation lines are permitted.

The output files for the SYVAC3-CC4 model listed in Table 5.5 include as a minimum the *.LPT file, the *.OUT output file, and the *.DOS file. Optional files include the parameter file *.PAR", the Time Series Package trace files *.SUB (geosphere), .NDS (biosphere) and *.CDS (vault).

5.1 INPUT FILE DESCRIPTION

The SYVAC3-CC4 input files are listed in Table 5.1.

5.1.1 Main Input File

The .INP input file consists of a sequence of fields, each consisting of a single number or a character string. The fields appear in consecutive logical records, which can be broken into shorter physical records, or lines, because the file is a Standard Text (ASCII) File. The input is broken into logical records to allow the use of optional fields, which may or may not occur. The fields in the main input file are described in general in Table 5.1. Appendix B contains an extraction from the complete median case SYVAC3-CC4 main ".INP" file created from the Horizontal Borehole Case Study database. This file used a QUANTILE sampling method for all parameters found in file "MEDIANHB.QNT".

This is an extraction because although all parameters (sampled, calculated, and consequence) are presented, parameters in arrays have been represented by the first and last entry of the array. Also, repetitive areas such as Element dependent and Nuclide dependent blocks that are grouped together to allow correct random sampling during a probabilistic simulation, are represented by their respective first and last blocks. This extraction was done to reduce the size of the file to a manageable volume but still provide information of all parameters in the main input file.

Table 5-1: Input Files for SYVAC3-CC4 Simulation

Input	Format	Contents
Terminal or batch File	Text, sequential,interactive	<ul style="list-style-type: none"> - identifying number of input file - new or restarted case
Main Input File (SVnn.INP)	Standard text file	<ul style="list-style-type: none"> - case title - input and output file options - simulation ranges requested - time series controls - INCLUDE file list - sampled parameters - dependent parameters - consequence parameters - nuclide list in chain order - matrix materials (wasteforms)
Model INCLUDE Files (SP*.INC, DP*.INC CQ*.INC)	Standard FORTRAN-77	<ul style="list-style-type: none"> - PARAMETER statements defining model-specific constants - common blocks containing model variables
Quantile Files (*QNT)	Standard text file (Optional file required for deterministic or controlled sampling simulations)	<ul style="list-style-type: none"> - lists of quantile values for parameters (=0.5 for Median Values)
Onfile Files (*ONF)	Standard text file (Optional file required for Deterministic or controlled sampling simulations)	<ul style="list-style-type: none"> - lists of actual values for parameters
Vault Solubility File (SOLnn.FXD)	Standard text file	<ul style="list-style-type: none"> - Fixed Nuclide Solubility Data
Geosphere Network File (NETnn.FXD)	Standard text file	<ul style="list-style-type: none"> - Fixed Network Parameter Data
Geosphere Sorption (SORnn.FXD)	Standard text file	<ul style="list-style-type: none"> - Fixed Sorption coefficient data
FRAC3DVS Control Input File (F3Dnn.FXD)	Standard text file	<ul style="list-style-type: none"> - FRAC3DVS data file name information - nuclide names - cross reference for FRAC3DVS slice label and geosphere discharge location
FRAC3DVS Data Input File (F3D_xxx_nn*.FXD)	Standard text file	<ul style="list-style-type: none"> - FRAC3DVS data

5.1.2 Simulation Control

Table 5.2 describes the fields that contain the simulation control information. These first four records or fields of the input file are the part of the file most likely to change from one case study to another. For example, if the model and the data set remain unchanged, and a different set of simulations is requested, that change would appear here. The user can select which optional files are produced from the input file, as shown in these tables. The three fields described as 4a, 4b, and 4c are used to define a range of simulations. They may be repeated many times in this record to describe multiple ranges.

Table 5-2: Simulation Control Information (INP File)

Record	Field	Type and Valid entries	Meaning
1	Case Title	Character*80; any string of ASCII characters.	The case title appears at the start of each SYVAC3 output file.
2	Output File Type	Character*5; 'LONG' or 'SHORT'	LONG' indicates that the value of every variable in every simulation should be stored in the OUT file; 'SHORT' means storage of only selected variables.
3	Optional Output File Extension	Character*3; 'PAR', 'SUB', 'NDS', 'CDS'	From 0 to 4 entries are allowed, separated by blanks, to indicate which optional files to produce. If 'PAR' is present, for example, then SYVAC3 will produce a file with the extension .PAR; otherwise it will not.
4a	First Simulation Number	Integer; $NF(1) > 0$, $NF(r+1) > NL(r)$, for $r > 0$	A range of simulations defines a sequence starting with NF and extending to NL. Simulations that lie within this range are to be performed in order.
4b	Number of Simulations Requested NR	Integer; $NR(r) > 0$, for all r	Simulations are to continue until either the number of "accepted" simulations reaches NR or the range is exhausted.
4c	Last Simulation Number NL	Integer; $NL(r) \geq NF(r)$, for all r	The Last Simulation Number must at least equal the First; there can be no empty ranges.

5.1.3 Time Series Controls

The fifth and sixth logical records in the input file provide Time Series controls that affect every Time Series generated in the application (Table 5.3). These controls specify the time frames of interest, and they affect the resolution of a Time Series in these time frames.

Table 5-3: Time Series Control Information (INP File)

Record	Field	Type and Valid entries	Meaning
5	Fixed Time	Double Precision. Can repeat from 1 to MXTFIX-1. Time entries should increase monotonically.	Every Fixed Time will appear in every Time Series. These times are also used to generate a mini-time series in the .OUT output file.
6a	Minimum Number of Time Steps: N_{min}	Integer; $2 < N_{min} \leq MXTSTP$	Each Time Series must hold at least this Number of times during the Time Series Construction stage; subsequently some may be deleted, and so this limit does not apply to the final form of a Time Series.
6b	Maximum Number of Time Steps: N_{max}	Integer $N_{min} \leq N_{max} \leq MXTSTP$	Each Time Series can hold no more than this Number of times in the final version, though more times may be used during the Time Series construction phase.
6c	Target Fractional Error, TFE	Double Precision $0.0 < TFE < 1.0$	SYVAC3 adds times to a Time Series Under Construction until the estimated fractional error in the area of the Time Series is less than the Target Fractional Error between each pair of consecutive Fixed Times.
6d	Time Smoothing Coefficient: St	Double Precision Optional: default is 0.20 $0 < St \leq 1$	Exponent used to transform times to a second scale on which each Time Series must be smooth.
6e	Value Smoothing Coefficient: Sr	Double Precision Optional: default is 0.20 $0 < Sr \leq 1$	Exponent used to transform values to a second scale on which each Time Series must be smooth.

The following guidelines should help the user to determine which settings to use:

- Fixed Times: Space some fixed times at regular intervals, either on a linear or a logarithmic scale depending on the time scale. Provide additional fixed times around the time when events of interest are occurring, but not too many (SYVAC3 will provide additional times as needed). Too many fixed times will slow execution time significantly. Note that these fixed time points are also used to generate a mini time series in the .OUT output file (see Section 6.5.3), independent of what SYVAC3-CC4 uses for internal calculations. If the user wants specific times to appear in this output time series, they must be specified in the fixed times.

- Minimum Number of Time Steps: Use a number such as 10 or 20. The objective in setting this entry is to ensure that the Time Series routines will find nonzero values in each Time Series. If this number is too small, a narrow nonzero part of a curve could be missed; if too large it could slow execution time.
- Maximum Number of Time Steps: This number is useful for controlling execution time. For a given Target Fractional Error, reducing this number will reduce execution time with relatively little impact on accuracy. Try starting with a value of about 200.
- Target Fractional Error (TFE): The Time Series routines in SYVAC3 can achieve a TFE as low as 0.001, meaning that the estimated area of a Time Series has about three correct significant figures. Execution times may be substantially reduced by using $TFE = 0.01$.
- Smoothing Coefficients: The Time Series package in SYVAC3 uses linear interpolation between points in a Time Series. Without smoothing (i.e., smoothing coefficient set to one) these look fine in linear plots, but plots of Time Series on a log-log scale look jagged. With smoothing coefficients set less than one, Time Series are constructed in such a way that they appear smooth on both linear and log scales. As a rule of thumb, use $1/(2M)$ for a smoothing coefficient, where M is the number of orders of magnitude to be shown on a log plot axis. For example, to show times from 10 to 100 000 years, use a Time Smoothing Coefficient of $0.125 = 0.5/(\log_{10} 100\,000 - \log_{10} 10)$. To show 20 orders of magnitude in values, use a Value Smoothing Coefficient of 0.025. Smaller values may cause numerical problems.

5.1.4 INCLUDE File List

The next section of the input file contains a list of all the SP* (sampled parameter), DP* (dependent parameter) and CQ*. INC (consequence parameter) INCLUDE files, one file name to a logical record. The number of INCLUDE files depends on the model, and so this section of the file is fixed for a given version of SYVAC3-CC4. The maximum number of common blocks that can be defined in INCLUDE files is 500 (MXCOM in SYVAC3). A record containing just the field 'END' marks the end of this section. SYVAC3 reads these files to find out where to get and store model variables in model common blocks. A file can contain declarations for more than one common block.

5.1.5 Sampling Methods

Four types of variables are shared between SYVAC3 and CC4, and three of them are listed in the input file: sampled parameters, dependent parameters and consequences. The fourth type of variable, Time Series, appears in the output files. The three variable types listed in the SYVAC3 input file can appear in any order and can be broken up into multiple groups. The total number of sampling methods (including the dependent and consequence types) is limited to MXSMTH=1000 in SYVAC3.

In each simulation, each sampled parameter takes a value sampled from a probability distribution provided by the input file. The sampling method determines how the sampled parameters are generated. All the parameters grouped together within one sampling method have their values assigned the same way. The supported sampling methods are:

- Random Sampling: A pseudorandom number generator produces a sequence of numbers uniformly distributed between zero and one, one for each parameter. This number is treated as a cumulative probability. It is transformed mathematically to a

value in the distribution that has that cumulative probability. For example, the cumulative probability 0.50 corresponds to the median of the distribution, whereas probabilities zero and one corresponds to the left and right extremes respectively. The only random sampling method prior to SV310 was 'RANDOM'. 'RANDOM 2' is a better generator, and each generator index guarantees an independent sequence of numbers, which was not true for 'RANDOM'.

- Quantile Sampling: A p-quantile of a distribution is a value with the cumulative probability p. Quantile sampling works like random sampling except that the p-values, which must lie between zero and one, are read from a file. The file name can contain up to MAXFNL characters (MAXFNL stands for MAXimum File Name Length). In SV311, MAXFNL is set to 32.
- On-File Sampling: Like the quantile sampling method, this one uses an auxiliary file. In the on-file method, the entries in the file are the actual parameter values. They may or may not lie within the bounds of the distribution in the input file. If they lie outside the bounds, the value is accepted, but a warning message is printed.

The files used for quantile and on-file sampling must be in standard ASCII format. Each must contain at least enough values in each logical record to assign one to each parameter using the sampling method.

Dependent parameters all appear in one or more sampling method groups each of which is labelled 'CALCULATED'. Consequences appear in one or more sampling method groups under the label 'CONSEQUENCES'. In each case there is one record per variable. These records establish the names, units and a few other attributes of each variable.

Table 5.4 shows one way an input file could be structured. The details of the records used to store data about the three types of variables are dealt with in subsequent sections. Note that the file includes two random methods, a quantile method and an on-file method. This means in any given simulation, some sampled parameters receive values from one pseudorandom sequence while others receive values from a different pseudorandom sequence, from a different pseudorandom number generator. Meanwhile other parameters receive values calculated from cumulative probabilities from input file VQINP.SMP, while others receive values directly from input file VOFINP.ONF.

5.1.6 Sample Files

Sample files provide values for sampled parameters in QUANTILE and ON-FILE sampling methods. QUANTILE sample files must provide numbers between zero and one. ON-FILE sample files may contain any set of appropriate parameter values. In both cases, all the values needed for a single simulation must appear in a single logical record. There must be as many records as simulations. These files are read as Standard ASCII Files, and so comments and continuation lines are permitted. An example sample file is provided in Appendix C.

Table 5-4: Example Sampling Method Layout for *.INP File (Note that all sampling methods need not be used in any given run)

Input File	Commentary
RANDOM' 61947329 ...<list of sampled parameters, one per record>... 'END'	61947329 is a random seed, used to initialize the pseudorandom number generator
'RANDOM 2' 7 ...<list of sampled parameters, one per record>... 'END'	7 is a generator index, used to specify one of $2^{32}-1$ independent generators.
'QUANTILE' 'VQINP.SMP' ...<list of sampled parameters, one per record>... 'END'	'VQINP.SMP' is the name of a Standard Text File containing cumulative probabilities.
CONSEQUENCES' ...<list of consequence variables, one per record>... 'END'	Consequence variables.
'ON FILE' 'VOFINP.ONF' ...<list of sampled parameters, one per record>... 'END'	'VQINP.ONF' is the name of a Standard Text File containing values of parameters.
'CALCULATED' ...<list of dependent parameters, one per record>... 'END'	Dependent parameters.
'CONSEQUENCES' ...<list of consequence variables, one per record>... 'END'	The second set of consequence variables is joined together internally with the first.
'END'	End of sampling methods.

5.1.7 Fixed Files

The fixed data input files contain data that are specific to a model such as the vault or geosphere in SYVAC3-CC4. In general these values do not change from simulation to simulation. For example, the fixed file input file for the vault solubility calculations are read in once during a simulation run even if multiple simulations are done within the same run.

The fixed files for SYVAC3-CC4 are the vault solubility file "SOLnn.FXD", the geosphere network file "NETnn.FXD", the geosphere sorption file "SORnn.FXD" and optionally the FRAC3DVS control input file "F3Dnn.FXD" and FRAC3DVS data files "F3D_xxx_nn.FXD" (Table 5.1).

Vault Solubility File

The vault nuclide solubility input data file contains data used to calculate nuclide solubility characteristics for U, Th, Pu, Tc, Np. The format of a typical input file is shown in Appendix D.

The solubility data file is read by the vault source code. The file contains 12 parameters, which must be in a specific order. Parameters IR1 and IR2 require one data entry each. Parameters IR1 and IR2 define ionic strengths. The remaining 10 parameters (P4, P5, P6, P7, P8, P9, P10, P2VLT, P3, and MNUM) are element and species dependent. Each of these parameters defines the number of complexing species associated with the 5 elements: uranium, thorium, technetium, plutonium, and neptunium. Each parameter-element combination can have zero or more entries, corresponding to the number of element species.

Geosphere Network File

The geosphere network file defines the layout of the geosphere transport network. Through this file, a simple or complex geosphere can be defined without any required code modification. An example of the complete network file is in Appendix E. This network is made up of nodes connected by one or more segments, which define the flow path of contaminants in the geosphere model from the vault source nodes through to the biosphere discharge nodes.

The CC408 geosphere model allows a maximum of 200 segments, 200 nodes, 10 biosphere discharge nodes, 25 vault source nodes, 20 different sorption minerals, 2 redox states of groundwater for each segment, 20 chemical property classes for segments, and 20 physical property classes for segments. If the maximum number of sources, discharge locations, nodes, or segment is not used, the remainder of each input section must be filled with zeroes. The network input file is made up of distinct input sections, as seen in Appendix E.

Geosphere Sorption File

An excerpt from the geosphere sorption input data file can be found in Appendix F. The format for the coefficients is given at the top of the file. Data for each element must begin with a character string of length 2 in uppercase. The element names must correspond in the correct order to elements given in the SYVAC3-CC4 main input file.

The CC4 geosphere model simulates a maximum of 25 elements, 20 sorbing minerals, and 2 groundwater redox states. Not all combinations of elements, minerals and redox states require input data. If a value is not required or not applicable to a particular mineral/redox combination, then all 10 coefficients are set to zero. In the excerpt from the sorption file, all the data for the first element in the input file "C" (carbon) has been listed. For all of the remaining elements, only the character string line used to identify the element has been left. Also included are the header lines for the dummy elements "DU" that are used as place holders to fill out the file.

FRAC3DVS Control Input File

Data from the code FRAC3DVS may be used instead of the CC4 calculated geosphere flows from the geosphere model. One control file and one or more data files must be present in the same run directory in order for FRAC3DVS data to be used. The control file provides information for the FRAC3DVS data file names along with nuclide names and a cross

references to the FRAC3DVS slice label and CC4 discharge locations which are to use the FRAC3DVS data. An example of a FRAC3DVS control input data file can be found in Appendix L.

FRAC3DVS Data Input File

Once a FRAC3DVS control input file is detected in the run directory, the data from the FRAC3DVS data files are read and geosphere flow time series are created, overwriting any CC4 calculated geosphere flows for that simulation. This file contains two comment lines at the beginning and is followed by the data, each line containing seven columns starting with the a FRAC3DVS slice label. Data for each slice label appears for one time point and is repeated for each of the next time points. For further information see an excerpt from a FRAC3DVS data input file in Appendix L.

5.2 OUTPUT FILE DESCRIPTION

The purpose of this section is to provide an overview of the output files produced by the SYVAC3-CC4 software program. The output files from a SYVAC3-CC4 simulation are listed in Table 5.5.

5.2.1 Time Series Files

The user can choose to print out the intermediate time series results. In essence, a time series approximates a parameter that changes with time as a series of (time, value) pairs. SYVAC3 provides many operations that can be performed on time series; among these is the "Write Time Series" operation that prints the (time, value) data into an ASCII format time series trace file. Each SYVAC3 time series operation that creates new time series invokes the "Write Time Series" operation automatically if a tracing flag within the code is set to TRUE (as it is within CC4.02).

SYVAC3 provides three optional files into which tracing information can go. Their extensions are .SUB, .NDS and .CDS. These extensions originally stood for SUBmodel output, Nuclide Dose Series and Combined Dose Series. When it became clear that some models were using these files in other ways, the definitions were downplayed, although the extensions remain. In the SYVAC3-CC4 model, the .CDS file is used for the vault model (INROC) time series, the .SUB is used for the geosphere model (GEONET) time series, and the *.NDS file for the biosphere model (BIOTRAC2) time series.

Time Series trace files can be quite large, since each Time Series representation can take tens to a few hundred lines. Usually trace files are produced for only a small number of simulations. However, a model could be designed to produce only a small number of time series in a trace file. The SHOWTS flag determines if time series for intermediate results should be written in the output file: setting SHOWTS=1 will limit the number of time series in the output file for the geosphere and biosphere submodels. That file could be used with a larger number of simulations. Also time series output can be removed out of the time series file using a standard ASCII editor. This file can be taken into a number of analysis packages such as Excel or S-Plus for presentation and analysis.

Vault (.CDS)

In order to fully understand the time series results for the vault model, one must trace or follow the generation of time series through the vault source code and the explanations given in the CC4 Theory Manual. Essentially the vault code produces the time series by first doing the general inventory and decay calculations, and then doing the transport analysis for each nuclide in the chain list order, and for each vault sector within the nuclide loop.

Geosphere (.SUB)

As with the vault time series, to fully understand the geosphere and biosphere time series results, one must follow the generation of time series through the geosphere or biosphere source code and the explanations given in the CC4 Theory Manual.

In general, the geosphere loops over a segment list, for each nuclide, passing flows from the segments directly connected to the vault source nodes up through the geosphere to the biosphere discharge nodes. After the transport simulation for each nuclide is completed, a summary is performed where the consequences are extracted for flow rates at selected nodes in the geosphere.

Biosphere (.NDS)

The biosphere calculations are based on a nuclide loop. The total dose curve is maintained as a running summation of all the nuclide doses calculated so far.

5.2.2 Parameter File (.PAR)

The parameter file is a fixed format text (ASCII) file that contains the values of all sampled (SP*.INC), dependent or calculated (DP*.INC), and consequence (CQ*.INC) parameters. The *.PAR file containing one line per variable, including constants. It shows the short name, long name, value and SI units for each variable. All the variables are listed for each simulation. The *.PAR file can be turned on or off by the user, and is usually only produced for cases with a small number of simulations, because this file can become very big (for large number of simulations, the *.OUT file is more compact). An example of the ".PAR" file format can be found in Appendix G.

This file has been treated in the same manner as the main SYVAC3-CC4 input file in that it contains excerpts from the main input file. For example, although all parameters are present, parameters in arrays have been represented by the first and last entry of the array. Also, repetitive entries such as Element dependent and Nuclide dependent blocks are represented by their first and last blocks. This extraction was done to reduce the size of the listing.

5.2.3 Dose File (.DOS)

The SYVAC3-CC4 model places in the DOS file

- the calculation order of the nodes of the geosphere network,
- a summary of the dose calculations performed in the biosphere, and
 - Maximum dose and time of maximum from all nuclides up to the time limit of the simulation;

- Maximum dose and time of maximum from all nuclides up to a user specified time in years;
 - Maximum total dose from each individual nuclide and time of maximum up to a user specified time in years;
 - Maximum total dose from each individual nuclide and time of maximum up to the time limit of the simulation;
- a table of maximum element concentrations in six of the biosphere model compartments.
 - Maximum chemical element concentration for each element for six biosphere compartments up to simulation time limit, and
 - Time of maximum chemical element concentration for each element for six biosphere compartments up to simulation time limit.

Appendix H contains the DOS file for a Horizontal Borehole Case Study median case simulation.

5.2.4 Compressed Output File (.OUT)

SYVAC3 always produces an OUT output file containing several kinds of information about a case of simulations. The SYVAC3 Version SV311 OUT file format is in ASCII format with a fixed record length (the previous version used a binary format). Details on the format of the OUT file can be found in Andres (2000).

Extraction of information can be accomplished using any text editor. However, SYVIEW and Perl scripts are used to extract information from the OUT file for analysis.

Once a dataset has been extracted from the OUT file, any suitable method (e.g., a statistics software package, a spreadsheet program, a graphical package) can be used to analyze and display the data.

5.2.5 System Output File (.LPT)

The line printer (LPT) file is a log of what happens during SYVAC3 execution. It begins with a copyright notice and file identification. It continues by echoing the input from the .INP input file. This information is formatted in such a way that the reader can better understand how SYVAC3 interpreted the input. It concludes by showing summaries of parameters, simulations, nuclide and time usage. Throughout, it records error and warning messages. Appendix I contains excerpts from the SYVAC3-CC4 median case .LPT file.

Table 5-5: Output Files for SYVAC3-CC4

Output File	Format	Contents
Terminal	Text, sequential,interactive	<ul style="list-style-type: none"> - copyright notice - case title - error and warning messages - simulation and timing summaries
Line Printer File (*.LPT)	Standard Text File - sequential - maximum record length=111 characters	<ul style="list-style-type: none"> - case title - copyright notice - input and output file options - simulation ranges requested - time series controls - INCLUDE file list for sampled, dependent and consequence parameters - nuclide list in chain order - matrix materials (wasteforms) - error and warning messages - simulation and runtime summary
Output File (*.OUT)	Standard Text File - maximum record length = 134 characters	<ul style="list-style-type: none"> - date and time - counts of variable types - sampling method random seeds or files - variable descriptions - constant parameter values - variable values for each simulation
Parameter Values File (*.PAR)	Standard Text File (optional) - sequential	<ul style="list-style-type: none"> - case title - date and time - variable values for each simulation
Time Series Trace Files (*.SUB, *.NDS, *.CDS)	Standard Text File (optional) - sequential - maximum record length =91 characters	<ul style="list-style-type: none"> - case title - date and time - for each time series recorded: time series headers, times and values, and area, error estimate and extremes
Model Output File (*.DOS)	Standard Text File	<ul style="list-style-type: none"> - case title - date and time - calculation order of geosphere nodes - peak total dose rate and time of peak - peak dose rate by nuclide and time of peak dose rate - dose rate by nuclide at 10,000 years

6. INDEX OF CC4 INPUT AND OUTPUT

This chapter presents the input and output parameters for the CC4.08 model. It is assumed that all parameters are "double precision real" unless otherwise indicated. A brief explanation is provided for parameters when the code definition may not suffice. Dimensioning parameters for all input parameters listed below are found in Section 2.8.2.

Input parameters occur in three types. One type of input parameters is supplied via the *.INP Input file and are known as "sampled parameters", since they are provided as a probability distribution that SYVAC3 then samples to obtain specific values for any given CC4 simulation. The second input type is supplied from a fixed data file, which is provided as single values and not as a probability distribution. The third type of input parameters are those calculated internal to CC4 by other models (e.g. calculated in vault and used in geosphere). The user must provide the first two classes of input, which are described in this chapter.

SYVAC3 output parameters are classed as either "dependent" or "consequence". In practice, dependent parameters typically are intermediate calculational results that may be of interest to the user, while consequence parameters are those final results of the simulation, such as maximum total dose rate to humans. These output parameters must be identified in the input file so that SYVAC3 knows which parameters to include in the *.PAR and *.OUT output files. The available output parameters are also listed in this chapter.

6.1 VAULT INPUT PARAMETERS

The vault model obtains user-supplied data through the *.INP file and the SOL*.FXD fixed data file. This fixed input file is used for five elements (U, Tc, Np, Pu and Th) whose solubility limits are calculated using thermodynamic relationships and a groundwater composition.

The vault input parameters are briefly discussed in the following sections and tables. They are organized by topic for clarity here. However, they are ordered in the input file itself as shown in Appendix B alphabetically in two groups – nuclide independent and nuclide dependent.

6.1.1 UO₂ Dissolution Rate Parameters

Degradation of the UO₂ fuel is driven by the presence of oxidative species created during radiolysis of the groundwater in the radiation field surrounding a fuel element or fragment. The radiolysis contributions of all types of radiation (alpha, beta, gamma) are considered plus a threshold chemical dissolution rate. The degradation rate of the fuel from each type of radiolysis is determined from empirical equations derived from the fitting of degradation rates. The parameters used for this calculation in the vault model are listed in Tables 6.1 to 6.3

6.1.2 Engineered System and Failed Container Parameters

The parameters used to represent the engineered system, including the characteristics of the failed container, are listed in Table 6.4. Note that the vault is divided into MAXSEC sectors, to allow for differences in vault design or behaviour across the vault (e.g. different local failure rates) and to allow for significant differences in the properties of the surrounding rock (e.g. groundwater flow rates). Parameters that can vary with sector are dimensioned by MAXSEC in

Table 6.4. The calculated contaminant release rate from each sector serves as a separate source term to a contaminant pathway through the geosphere.

6.1.3 Radionuclide Parameters

Table 6.5 lists the input parameters that describe the nuclide (or species) dependent properties such as half-life. Nuclides in each matrix material (i.e., UO₂ fuel or Zircaloy cladding) are treated as separate species. This allows for different properties such as inventories and instant release fractions for nuclides such as ¹⁴C_{FUEL} and ¹⁴C_{ZRLY}.

6.1.4 Buffer/Backfill Sorption Parameters

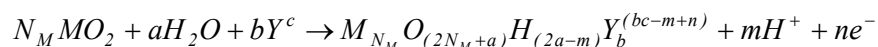
The sorption rates for elements in the buffer and backfill are listed in Table 6.6. Input parameters that are element specific are dimensioned by MXCHEM. The number of elements in a simulation must be less than or equal to the number of nuclides in a simulation. Each element listed must correspond to at least one nuclide.

6.1.5 Solubility Parameters

The solubility of a nuclide is based on the solubility of the underlying chemical element. When there are multiple isotopes of the same element present in the same wastefrom, they are each assigned a proportional share of the total elemental solubility. The solubility of most elements is a user input via the MAXSOL parameter per Table 6.7. These solubility limits are applied inside the container, so should be chosen to be representative of conditions at this location.

However, if the parameter SOLOPT = 1 (Table 6.7), then the solubilities of five elements - U, Np, Pu, Th and Tc - are calculated from groundwater composition and chemical reaction constants listed in Table 6.7.

The chemical reactions themselves are described through the file SOL*.FXD, with the parameters listed in Table 6.8. These input parameters are not sampled from a probability distribution, but are used directly. The reactions are written in the form:



where $M_{N_M} O_{(2N_M+a)} H_{(2a-m)} Y_b^{(bc-m+n)}$ is an aqueous solution species and Y^c is a complexing ligand with ionic charge c . The input parameters that describe these reactions are: P2VLT = m , P3 = n , MNUM = N_M (Table 6.8) and P4-P10 are the b values for Y^c = carbonate, phosphate, sulphate, chloride, fluoride and two organic complexing ligands, respectively.

6.1.6 Vault Transport Parameters

The parameters used to define the transport processes in the vault are listed in Table 6.9.

6.2 GEOSPHERE INPUT PARAMETERS

6.2.1 Segment Dependent Parameters

The geosphere is divided up into physical property class zones. Within these zones, segments are assumed to have similar physical properties. The segment dependent input parameters for the geosphere model are listed in Table 6.10. Some of the properties are assigned through the physical property class and some segment-by-segment.

6.2.2 Node Dependent Parameters

The node dependent input parameters for the geosphere model are listed in Table 6.11.

6.2.3 Well Parameters

The well input parameters for the geosphere model are listed in Table 6.12.

6.2.4 Geosphere Network

The fixed network data parameters for the geosphere model, found in the fixed data file for the network (NET*.FXD), are listed in Table 6.13 and Table 6.14 for segment and nodal properties respectively. These provide the links between the nodes and segments in the geosphere, and the corresponding interfaces with the vault sectors and the biosphere discharge zones.

6.2.5 Geosphere Sorption Parameters

The fixed sorption parameters, found in the fixed data file for sorption (SOR*.FXD), for the geosphere model are listed in Table 6.15.

6.2.6 Chemical Property Dependent Parameters

The geosphere is divided up into chemical property class zones. Within these zones, segments are assumed to have similar chemical properties. The chemical property class parameters for the geosphere model are listed in Table 6.16.

6.2.7 Geosphere/Biosphere Interface Parameters

The input parameters that define the discharge zones from the geosphere to the biosphere are listed in Table 6.17. Each discharge zone may have an overburden and (then) a sediment (or saturated soil) layer between the bedrock and the surface discharge point.

6.2.8 Water Properties

Input parameters that define the properties of water are listed in Table 6.18.

6.2.9 Glaciation State Parameters

Input parameters associated with glaciation are listed in Table 6.19.

6.3 BIOSPHERE INPUT PARAMETERS

6.3.1 Surface Water Parameters

The parameters that describe the surface waters (i.e., lake, precipitation) are listed in Table 6.20.

6.3.2 Soil

The soil and lake sediment model parameters are listed in Table 6.21.

6.3.3 Atmosphere

The parameters used in the atmosphere model for transport in the biosphere model are listed in Table 6.22.

6.3.4 Concentrations in Plants and Animals

The parameters used to determine the concentrations in plants and animals in the biosphere model transport model are listed in Table 6.23.

6.3.5 Radiation Exposure for Reference Humans and Animals

The parameters used to determine the radiation exposure to the reference human group and reference biota include uptake or exposure rates, hold up times, occupancy rates, and pathway specific parameters. The input parameters that provide this information have been grouped into relevant tables as detailed below:

- Table 6.24, reference human group lifestyle characteristics.
- Table 6.25, human ingestion and inhalation rate data.
- Table 6.26, animal ingestion and inhalation rate data.
- Table 6.27, doses from plant sources.
- Table 6.28, occupancy factors used for building, ground, humans, non-humans, and water immersion.
- Table 6.29, holdup times used for the various pathways. These holdup times represent the time a radionuclide is held or built up in the specific vector for the dose calculations.
- Table 6.30, human dose coefficients.
- Tables 6.31 to 6.34, some elements (C, Cl, H, and I) have additional parameters used in the determination of the dose estimates.

6.3.6 Radiation Exposure for Non-Human Biota

Dose coefficients used for the generic target plant, mammal, bird and fish are presented in Table 6.35.

6.3.7 Other Input Parameters

Table 6.36 lists other input information provided in the *.INP input file.

In the biosphere model, the consequence results are limited to the maximum concentration CNLIM.

Certain dose rate time series information is output to the *.OUT/*.PAR files at the LTIM time points.

Several unit conversion rates are defined in the input file (to avoid hardwired parameters).

6.4 DEPENDENT PARAMETERS

The values of dependent parameters are assigned before any time-dependent calculations are performed. These values are printed in the PAR and OUT output files.

6.4.1 Vault Dependent Parameters

The vault model dependent parameters are calculated from values stored in the vault sampled parameter variables or other dependent parameters. Table 6.37 lists all dependent parameters calculated by the vault model. Table 6.37 contains the parameters that are calculated by the geosphere model and passed to the vault.

6.4.2 Geosphere Dependent Parameters

The geosphere model dependent parameters used for calculations within the geosphere model are presented in Table 6.38. This table contains the dependent parameters that are indexed by node, segment and property class.

6.4.3 Geosphere/Biosphere Interface

The geosphere/biosphere model interface mainly passes information regarding the discharge locations. The discharge and well model dependent parameters are listed in Table 6.39.

6.4.4 Geosphere/Vault Interface

The Geosphere/Vault interface parameters are listed in Table 6.40. This table lists the parameters determined in the geosphere that are required by the vault model.

6.4.5 Biosphere Dependent Parameters

The dependent parameters defined and used in the biosphere model are presented in three tables as follows:

- Table 6.41, biosphere transport model.
- Table 6.42, biosphere dose model.
- Table 6.43, biosphere irrigation model.

6.5 CONSEQUENCES PARAMETERS

Consequence parameters are initialized to zero. However if a simulation is not accepted, SYVAC3 assigns an artificial value to all consequence parameters, typically -1.

6.5.1 Vault Consequences

All consequence parameters produced by the vault model are listed in Table 6.44.

6.5.2 Geosphere Consequences

All consequence parameters produced by the geosphere model are listed in Table 6.45. If the maximum number of geosphere consequences, MXGCNQ, is exceeded, the geosphere consequences are written to the simulation log file (.LPT).

6.5.3 Biosphere Consequences

All consequence parameters produced by the biosphere model are listed in this section.

The maximum total dose rate to man and time of maximum total dose rate are listed in Table 6.46. The maximum total dose rate represents the total dose for all nuclides and all pathways combined. This maximum is determined for two time ranges. The first range is from the start of the simulation up to 10,000 a, the second is again from the start of the simulation but out to the time limit of the simulation. This table also lists the consequence parameter VALDA. This parameter is used to represent a subseries of the final total dose rate time series for "NLTIM" values. The time points for this time series are selected based on the fixed times provided in the input file. If the user wants specific times to appear in the time series, they must be specified in the fixed times. If there are less than NLTIM fixed times, then the code will calculate times to fill the list. If there are more than NLTIM fixed times, then the fixed times near the beginning of the fixed time list will not be included in the output. (Note that this output time series is independent of that used internally by SYVAC3-CC4 for calculations.)

The total dose for all pathways per nuclide simulated is presented in Table 6.47. As in Table 6.46, the maximum value and time of maximum are reported for two time ranges. The peak dose rates are given for each pathway and nuclide for the time of maximum dose rate per nuclide for all pathways combined.

The parameters for integrated nuclide dose for each pathway and the nuclide order are presented in Table 6.48. Table 6.48 also describes the consequence parameter "VALDT".

The maximum total dose rate and time of maximum total dose rate to non-human biota are listed in Table 6.49. These values are determined for two time ranges as was done for the parameters in Table 6.46. Also listed in Table 6.49 is "VALDNA", this is similar to the parameter "VALDA" in Table 6.46, a subseries of the final total dose rate time series for "NLTIM" values.

The peak and maximum nuclide dose rates are listed in Table 6.50. The peak dose rates are given for each pathway and nuclide for the time of maximum dose rate per nuclide for all pathways combined. This is done for each type of non-human biota (bird, fish, mammal, and plant). A subseries of the dose rate time series for each nuclide and type non-human biota is also listed.

The biosphere model determines the maximum concentration and time of maximum concentration for each nuclide and a set of twelve biosphere compartments (Table 6.51). These compartments include four field compartments (vegetable patch, forage field, woodlot, and peat bog), four sediments compartments (vegetable patch, forage field, woodlot, and peat bog), two

water compartments (lake and well), and two air compartments (indoor and outdoor). The total chemical element concentration and time of maximum concentration for each element is calculated in six biosphere compartments namely, lake water, well water, soil, lake sediment, indoor air and outdoor air (Table 6.51). Two safety indicators are also calculated: 1) the maximum value of the total radiotoxicity flux for all nuclides from the geosphere to the biosphere as well as the time this maximum occurs and 2) the maximum value of the total radiotoxicity concentration for all nuclides in lake water as well as the time this maximum occurs (Table 6.51). Table 6.51 also lists the mass accumulation parameters for the biosphere.

Table 6.52 provides a listing of the maximum and time of the maximum for the activity/concentration values for the simulated radionuclides/non-radionuclides. To be specific, a radionuclide will have an activity value whereas a non-radionuclide will have a concentration.

The consequence parameters found in Table 6.53 are used to indicate the status of the biosphere model after a simulation. The flags or informational indexes are used to indicate the water source (0=NONE,1=LAKE,2=WELL) for the specified field (vegetable patch, forage field, woodlot, and peat bog).

The warning parameters in Table 6.54 are set when an internal limit of the biosphere model has been exceeded. When one of these limits is exceeded the appropriate flag is set equal to "1". This table also includes two parameters that give the time that the groundwater dilution limit was exceeded for both the critical group and nonhuman biota.

6.5.4 Mass Accumulation and Distribution Consequences

The mass accumulation and distribution consequence parameters produced by all the submodels are listed in Table 6.55.

Table 6-1: Used Fuel Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
DGRYP	matrix degradation process or type []	MXMTRX	SPDEGR
RUCHEM	chemical fuel dissolution rate [mol/(m ² .a)]	scalar	SPGAMA
TCOOL	Age of fuel at start of calculations [a]. Note: The dose rate data (ALPHDO, BETADO, GAMADO) start at reactor discharge, but the initial nuclide inventories (INVPKG) are at start of calculations.	scalar	SPRADI
TMDSSL	time for complete dissolution of metal wastefrom [a]	MXMTRX	SPINVT
USURFA	Effective surface area of used fuel per container [m ²]	scalar	SPRADI
WASTCO	mass of wastefrom in each container [kg]	MXMTRX	SPINVT

Table 6-2: Alpha Radiolysis Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AALPHA	exponent for dependence of fuel dissolution rate on the alpha radiolysis dose rate []	scalar	SPALPH
ALFCOF	uncertainty factor in alpha dose rate to used fuel []	scalar	SPALPH
ALPHDO	values of alpha dose rate to the surface of used fuel [Gy/a]	MXUDOS	SPALPH
ALPHTI	time values for alpha dose rate to the surface of used fuel [a]	MXUDOS	SPALPH
GALPHA	rate constant for fuel dissolution due to alpha radiolysis [mol.m ⁻² .Gy ⁻¹]	scalar	SPALPH
NOALPH	number of entries in alpha dose time series []	scalar	SPALPH

Table 6-3: Beta and Gamma Radiolysis Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
ABETA	exponent for dependence of fuel dissolution rate on the beta radiolysis dose rate []	scalar	SPBETA
AGAMMA	exponent for dependence of fuel dissolution rate on the gamma radiolysis dose rate []	scalar	SPGAMA
BETADO	values of beta dose rate to the surface of used fuel [Gy/a]	MXUDOS	SPBETA
BETATI	time values for beta dose rate to the surface of used fuel [a]	MXUDOS	SPBETA
BETCOF	uncertainty factor in beta dose rate to used fuel []	scalar	SPBETA
GAMADO	values of gamma dose rate to the surface of used fuel [Gy/a]	MXUDOS	SPGAMA
GAMATI	time values for gamma dose rate to the surface of used fuel [a]	MXUDOS	SPGAMA
GAMCOF	Ratio of gamma dose rate in container to dose rate at surface of a single used fuel bundle []	scalar	SPGAMA
GBETG	rate constant for fuel dissolution due to beta or gamma radiolysis [mol.m ⁻² .Gy ⁻¹]	scalar	SPBEGA
NOBETA	number of entries in beta dose time series []	scalar	SPBETA
NOGAMA	number of entries in gamma dose time series []	scalar	SPGAMA

Table 6-4: Engineered System and Failed Container Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
IFAILQ	instant container failure quantile []	MAXSEC	SPIFLQ
IFRACT	instant failure fraction []	scalar	SPCNF1
LENCHO	length of hole in container [m]	scalar	SPTHCK
LENROM	length of disposal room [m]	MAXSEC	SPTHCK
NCONSC	number of containers per sector []	MAXSEC	SPCONS
PORCON	infiller capacity factor []	scalar	SPVLT
PORDAM	porosity of damaged zone []	scalar	SPVLT
PORHOL	porosity for inside the hole in the container []	scalar	SPVLT
RADCHO	radius of hole in container [m]	MAXSEC	SPTHCK
RMANGL	angle of disposal room axis with geosphere x-direction [deg]	scalar	SPVLT
ROMSPA	centre to centre room spacing [m]	scalar	SPTHCK
TDELAY	time delay between closure of the repository and exposure of the waste to groundwater [a]	MAXSEC	SPDELY
TEMPSC	vault reference temperature [K]	scalar	SPTMPS
THKBAK	effective thickness of backfill [m]	scalar	SPTHCK
THKBUF	effective thickness of buffer [m]	scalar	SPTHCK
THKDAM	effective thickness of damaged zone [m]	scalar	SPTHCK
VOLUMC	internal volume of container [m ³]	scalar	SPVLT

Table 6-5: Nuclide Dependent Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
HLIFE	Half-life of each radionuclide [a] Note: Stable nuclides must have a half-life greater than or equal to MXHLIF. Radionuclides with a half-life less than MNHLIF are not simulated.	MXSPEC	SPHALF
INVPKG	initial nuclide inventories [mol/kg]	MXSPEC	SPINVT
IRFRAV	instant release fraction for each nuclide []	MXSPEC	SPIRFR

Table 6-6: Buffer/Backfill Sorption Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CAPBFE	element capacity factors in buffer []	MXCHEM	SPCAPF
CAPBKE	element capacity factors in backfill []	MXCHEM	SPCAPF

Table 6-7: Solubility Fixed Input Parameters (SOL*.FXD File)

Parameter	Definition [Units]	Dimension	Common Block
IR1	first reference ionic strength []	scalar	FPRION
IR2	second reference ionic strength []	scalar	FPRION
MNUM	number of metal atoms in reaction []	MAXELM, MAXSPE	FPMNUM
P2VLT	pH solubility parameter []	MAXELM, MAXSPE	FPSOLP
P3	Eh solubility parameter []	MAXELM, MAXSPE	FPSOLP
P4	carbonate index []	MAXELM, MAXSPE	FPINIX
P5	HPO ₄ ⁻² index []	MAXELM, MAXSPE	FPINIX
P6	sulphate index []	MAXELM, MAXSPE	FPINIX
P7	chloride index []	MAXELM, MAXSPE	FPINIX
P8	fluoride index []	MAXELM, MAXSPE	FPINIX
P9	first organic index []	MAXELM, MAXSPE	FPORIX
P10	second organic index []	MAXELM, MAXSPE	FPORIX

Table 6-8: Solubility Input Parameters (INP File)

Parameter	Code Description [Units]	Dimension	Common Block
CCARBT	total solution carbonate []	scalar	SPMICN
COL1	organic ligand 1 concentration []	scalar	SPCORL
COL2	organic ligand 2 concentration []	scalar	SPCORL
CFTOT	fluoride concentration []	scalar	SPMICN
CPTOT	inorganic phosphorus concentration []	scalar	SPMICN
CCACL2	calcium chloride concentration []	scalar	SPMJCN
CNACL	sodium chloride concentration []	scalar	SPMJCN
CNASUL	sodium sulphate concentration []	scalar	SPMJCN
ETCA	TcO ₂ /TC potential Ph=0 [V]	MAXIFI	SPETBD
ETCB	temperature dependence of TcO ₂ /TC potential [V/K]	scalar	SPETBD
EUO3A	UO ₂ /UO ₃ potential at PH=0 [V]	MAXIFI	SPEUBD
EU03B	temperature dependence of UO ₂ /UO ₃ potential [V/K]	scalar	SPEUBD
EZI	initial reference potential for system [V]	scalar	SPSPOT
KCASLR	log of CaSO ₄ solubility product at 298 K []	MAXISI	SPLOGC
KCASLS	Temp. dependence of CaSO ₄ solubility product [1/K]	scalar	SPSLTD
KP2S	Temp. dependence of 2nd PO ₄ protonation constant [1/K]	scalar	SPSLTD
KS1S	Temp. dependence of 1st CO ₃ protonation constant [1/K]	scalar	SPSLTD
KP2R	log of 2nd PO ₄ protonation constant at 298 K []	MAXISI	SPLOGC
KS1R	log of 1st CO ₃ protonation constant at 298 K []	MAXISI	SPLOGC
KS2R	log of 2nd CO ₃ protonation constant at 298K []	MAXISI	SPLOGC
KSCR	log of CaCO ₃ solubility product at 298 K []	MAXISI	SPLOGC
KSFR	log of CaF ₂ solubility product at 298 K []	MAXISI	SPLOGC
KSPR	log of hydroxyapatite solubility product at 298 K []	MAXISI	SPLOGC
KS2S	temp. dependence of 2nd CO ₃ protonation constant [1/K]	scalar	SPSLTD
KSCS	temp. dependence of CaCO ₃ solubility product [1/K]	scalar	SPSLTD
KSFS	temp. dependence of CaF ₂ solubility product [1/K]	scalar	SPSLTD
KSPS	temp. dependence of hydroxyapatite solubility product [1/K]	scalar	SPSLTD
KWS	temp. dependence of water ion product [1/K]	scalar	SPSLTD
KWR	log of water ion product at 298 K []	MAXISI	SPLOGC

continued...

Table 6-8: Solubility Input Parameters (INP File) (concluded)

Parameter	Code Description [Units]	Dimension	Common Block
MAXSOL	maximum solubility of an element [mol/kg]	MXCHEM	SPMXSL
NS	number of solubility species reactions for an element []	MAXELM	SPNSL
P1R	log K at 298 K for solubility species reactions []	MAXIFI, MAXELM, MAXSPE	SPECON
P1S	Temp. dependence of equilibrium constant for solubility species reactions [1/K]	MAXELM,MAX SPE	SPECON
PH	pH []	scalar	SPPH
SLP25	Eh S factor at 25 C [V]	scalar	SPSL25
SOLOPT	Indicates solubility calculation; SOLOPT = 0 use MAXSOL for all elements, SOLOPT =1 use calculated value.	scalar	SPCSOL

Table 6-9: Vault Transport Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
BKPERM	Backfill permeability [m ²]	scalar	SPBACK
DIFBAK	total intrinsic diffusion coefficient in backfill [m ² /a]	MXCHEM	SPDIFF
DIFBUF	total intrinsic diffusion coefficient in buffer [m ² /a]	MXCHEM	SPDIFF
DIFCHO	total intrinsic diffusion coefficient for inside hole in container [m ² /a]	MXCHEM	SPDIFF
DZPERA	damaged zone permeability parallel to the axis of the disposal room [m ²]	scalar	SPBACK
LEDBAK	axial dispersion length for backfill [m]	scalar	SPTHCK
LEDDAM	axial dispersion length for damaged zone [m]	scalar	SPTHCK
LETBAK	axial transverse dispersion length for backfill [m]	scalar	SPTHCK
LETDAM	axial transverse dispersion length for damaged zone [m]	scalar	SPTHCK
RAPERD	ratio of transverse to axial permeability for damaged zone []	scalar	SPBACK
RAPERZ	ratio of damage zone permeability parallel to the axis of the disposal room and the permeability on the host rock []	scalar	SPBACK
RARDAM	ratio of radial to axial dispersion length for damaged zone []	scalar	SPTHCK
RATDAM	ratio of radial to axial transverse dispersion length for damaged zone []	scalar	SPTHCK
TORDAM	tortuosity of damaged zone []	scalar	SPVLT

Table 6-10: Geosphere Segment Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
SGDSPF	dispersion length factor []	MAXSEG	SPSEG1
SGGWVI	segment groundwater velocity input [m/a]	MAXSEG	SPSEG1
SGHYCO	hydraulic conductivity [m/a]	MAXSEG	SPSEG1
SGPERM	permeability [m ²]	MAXSEG	SPSEG2
SGSFRI	initial source fraction []	MAXSEG	SPSEG2
SGTFRL	transfer length [m]	MAXSEG	SPSEG2
SGFAPT	effective aperture of fractures [m]	MXPPCL	SPSEG3
SGFSPA	effective spacing of fractures [m]	MXPPCL	SPSEG3
SGPROS	total porosity []	MXPPCL	SPSEG3
SGRETM	factor for retardation in matrix []	MXPPCL	SPSEG3
SGTORA	axial tortuosity []	MXPPCL	SPSEG3
SGTORM	matrix diffusion tortuosity []	MXPPCL	SPSEG3
VSCALE	scaling factor for groundwater velocities []	scalar	SPSEG1

Table 6-11: Geosphere Node Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
NDHEAD	node reference hydraulic head in absence of well [m]	MAXNOD	SPNODS
NDPOSX	node position, x-coordinate [m]	MAXNOD	SPNODS
NDPOSY	node position, y-coordinate [m]	MAXNOD	SPNODS
NDPOSZ	node position, z-coordinate [m]	MAXNOD	SPNODS
NDTEMP	node temperature [°C]	MAXNOD	SPNODS

Table 6-12: Well Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
DISCC1	well bypass discharge eqn C1 [a/m^3]	scalar	SPWELL
DISTD1	distance to 1st drawdown node [m]	scalar	SPWELL
DISTD2	distance to 2nd drawdown node [m]	scalar	SPWELL
DPTHWL	well depth below water table [m]	scalar	SPWELL
NAQDA1	nonaquifer drawdown eqn A1 [a/m^5]	MAXNOD	SPWELL
QSCALE	scaling factor for well demand []	scalar	SPWELL
RADWEL	radius of well casing [m]	scalar	SPWELL
THIKAQ	thickness of well aquifer [m]	scalar	SPWELL

Table 6-13: Geosphere Fixed Segment Input Parameters (NET*.FXD File)

Parameter	Definition [Units]	Dimension	Common Block
GWVFID	groundwater velocity input indicator: [] 1 = velocity input; 2 = Darcy vel input, linear velocity calculated. 3 = hyd. conductivity input, velocity calculated; 4 = head and permeability input, both hyd. conductivity and velocity calculated; 5 = head, permeability and temperature input, both hyd. conductivity and velocity calculated; 6 = head, permeability and temperature input, both hyd. conductivity and velocity calculated using buoyancy terms;	scalar	FPSEGS
SGCPCL	chemical property class []	MAXSEG	FPSEGS
SGNODI	input node number []	MAXSEG	FPSEGS
SGNODO	output node number []	MAXSEG	FPSEGS
SGPPCL	physical property class []	MAXSEG	FPSEGS
SGRFID	Boundary condition identifier: [] 1 = semi-infinite medium; 2 = mass transfer coefficient; 3 = zero concentration b.c.; 4 = flow passed unchanged; 5 =MULTIC, compartment model mimic a semi-infinite b.c.; 6 =MULTIC, compartment model mimic a zero concentration b.c.	MAXSEG	FPSEGS
SGTLIK	Segments that are in open talik passing through permafrost	MAXSEG	FPSEGS
STPFTL	code number for glaciation state permafrost-talik presence: 0 = no frozen ground, no talik possible; 1 = frozen ground (permafrost) but no open talik; 2 = frozen ground (permafrost) with open talik	MXGSTA	FPGLAC

Table 6-14: Geosphere Fixed Node Input Parameters (NET*.FXD File)

Parameter	Definition [Units]	Dimension	Common Block
NODEA	node list for well aquifer nodes []	MAXNOD	FPNODE
NODEB	node list for biosphere discharges []	MAXLOC	FPNODE
NODEC	node list for consequences []	MAXNOD	FPNODE
NODEO	node list for calculation order of output nodes []	MAXNOD	FPNODE
NODES	node list for source nodes []	2*MAXSEC	FPNODE
NODEV	node list for vault nodes which are affected by well drawdown []	MAXNOD	FPNODE
NODWL	well lower reference node []	scalar	FPNODE
NODWU	well upper reference node []	scalar	FPNODE
SECNO	vault sector numbers connected to each source node []	2*MAXSEC	FPNODE
TYPNOD	code number for type of biosphere discharge []	MAXLOC	FPNODE
TYPSEC	code number for type of vault release []	2*MAXSEC	FPNODE

Table 6-15: Sorption Fixed Input Parameters (SOR*.FXD File)

Parameter	Definition [Units]	Dimension	Common Block
SORC00	coefficient for constant Kd term [L/kg]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC01	coefficient for linear term in salinity [L/kg]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC02	coefficient for linear term in nuclide concentration [L/kg]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC03	number of orders of magnitude of variation in calculated Kd []	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC04	geometric mean of nuclide concentration [mol/L]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC05	number of orders of magnitude of variation in nuclide concentration []	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC06	normalization factor to give contribution to retardation factor [kg/L]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC11	coefficient for quadratic term in salinity [L/kg]	MXMNRL, MXOXST, MXCHEM	SORDAT
SORC12	coefficient for cross-term in salinity and nuclide concentration [L/kg]	MXOXST, MXMNRL, MXCHEM	SORDAT
SORC22	coefficient for quadratic term in nuclide concentration [L/kg]	MXOXST, MXMNRL, MXCHEM	SORDAT

Table 6-16: Chemical Property Dependent Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CNRAER	uncertainty factor for concentration, logarithmically distributed in range (0.1,10.0) []	MXMNRL, MXCHEM	SPCNER
COLLKD	sorp coeff for element on colloid [L/kg]	MXCHEM	SPCOLL
COLLRT	colloid retardation factor []	MXCPCL	SPCOLL
DIFFN	free water diffusion constant of element [m ² /a]	MXCHEM	SPDIFN
ELOXDV	depth of redox divide [m]	scalar	SPWCHM
KDRAER	error factor for Kd, logarithmically distributed in range (0.1,10.0) []	MXMNRL, MXCHEM	SPKDER
SGCOLL	concentration of colloids [kg/L]	MXCPCL	SPCOLL
SGMNRL	fractional mineral content []	MXMNRL, MXCPCL	SPRCHM
SGSALN	salinity of groundwater [kg/m ³]	MXCPCL	SPWCHM

Table 6-17: Geosphere/Biosphere Interface Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AREAD	Area of discharge [m ²] Note: Set to total (aquatic plus terrestrial) discharge area for aquatic discharges, and ignored for terrestrial discharge. Aquatic/terrestrial split set via DISFRA.	MAXLOC	SPAREA
DISFRA	Fraction diverted to discharge []	MAXLOC	SPDSFR
THIKOV	thickness of overburden layer [m]	MAXLOC	SPSSOV
THIKSS	thickness of sediment layer [m]	MAXLOC	SPSSOV

Table 6-18: Water Property Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
COMWAT	compressibility of water [Pa^{-1}]	scalar	SPWATR
DENA	coefficient A for water density equation [K^{-1}]	scalar	SPWATR
DENB	coefficient B for water density equation [K^{-2}]	scalar	SPWATR
DENREF	density of water at 6°C [kg/m^3]	scalar	SPWATR
RHO0	density of water at 25°C [kg/m^3]	scalar	SPWATR
TEM0	reference temperature for RHO0 [°C]	scalar	SPWATR
VISA	coefficient A for water viscosity eqn [$\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$]	scalar	SPWATR
VISB	coefficient B for water viscosity eqn [K]	scalar	SPWATR
VISREF	viscosity of water at 6°C [$\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$]	scalar	SPWATR

Table 6-19: Geosphere and Biosphere States Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
DCMPT	number of compartments []	Scalar	SPSTAT
ELIZBS	elevation of immobile zone basement [m]	MXGSTA	SPSTAT
BIDXS	cross reference index from periods to states for biosphere []	MAXPER	SPSTAT
GIDXS	cross reference index from periods to states for geosphere []	MAXPER	SPSTAT
GSCALE	scaling gw flow for geosphere states []	MAXSEG, MXGSTA	SPSTAT
TDURAT	time period duration [a]	MAXPER	SPSTAT

Table 6-20: Surface Water Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AREAAQ	lake surface area [m^2]	MXBSTA	SPLAKE
AREATE	catchment area of watershed [m^2]	MXBSTA	SPLAKE
LD	mean depth of the surface water body [m]	MXBSTA	SPLAKE
MLTWTR	meltwater production [m/a]	MXBSTA	SPLAKE
RUNOFF	watershed average runoff (P-ET) [m/a]	MXBSTA	SPLAKE
PRECIP	total annual precipitation (P) [m/a]	MXBSTA	SPPPTN

Table 6-21: Soil and Lake Sediment Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
DPSTYP	surface soil layer soil type []	scalar	SPSTYP
FLRALS	effective loss rate from surface soil due to flora and fauna related soil turbation [m/a]	scalar	SPRNFD
LAYRR	depth of the surface soil layer [m]	MXBSTA	SPSOIL
LCHFAC	leaching rate fraction for upland soils []	MXBSTA	SPSOIL
LPARTM	rate of deposition of lake sediments [kg/(m ² .a)]	scalar	SPLAKE
MOIST	surface soil moisture content [m ³ /m ³]	NSOIL	SPSOIL
NFBS	exponent for groundwater effective upflow rate []	scalar	SPRNFD
NSED	thickness of new sediment [m]	scalar	SPTSED
PROSED	indicates whether sediment is used as soil; No = 0, Yes = 1 []	MXBSTA	SPSSWT
QIRR	field irrigation demand [m/a]	MXFELD, NSOIL, MXBSTA	SPQIRR
RNOFFD	inflow of uncontaminated water into discharge from adjacent areas [m ³ /a]	MAXLOC	SPRNFD
SD	depth to water table [m]	MXBSTA	SPSOIL
SBD	surface soil bulk density [kg/m ³]	NSOIL	SPSOIL
SDLOW	minimum depth to water table for upland soil model (otherwise use shallow soil model) [m]	scalar	SPSOIL
SEDBD	sediment bulk density [kg/m ³]	scalar	SPLAKE
SEDSOR	rate of removal of nuclide from lake water to the sediment [1/a]	MXCHEM, MXBSTA	SPLAKE
SKD	radionuclide distribution coefficient in surface soil [L/kg]	MXCHEM, NSOIL	SPSOIL
THSED	thickness of accessible sediment in lake [m]	scalar	SPTSED
WSD	water summer deficit in surface soil [m/a]	scalar	SPRNFD

Table 6-22: Atmosphere Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AADL	atmospheric dust (aerosol) load from the lake [m ³ /m ³]	scalar	SPATMS
ADLT	atmospheric dust load from the soil [kg/m ³]	scalar	SPATMS
BLDHT	building height [m]	MXBSTA	SPATMS
BLDWI	building width [m]	MXBSTA	SPATMS
CLEFRQ	frequency of land clearing fires [1/a]	MXBSTA	SPATMS
DEGASL	rate constants for loss of gaseous nuclides from lake by degassing [1/a]	MXCHEM, MXBSTA	SPDGAS
DEGASS	rate constant for loss of nuclide from soil by degassing [1/a]	MXCHEM, NSOIL, MXBSTA	SPDGAS
DISA1	term 1 for aqueous dispersion function []	scalar	SPATMS
DISA2	term 2 for aqueous dispersion function []	scalar	SPATMS
DIST1	term 1 for terrestrial dispersion function []	scalar	SPATMS
DIST2	term 2 for terrestrial dispersion function []	scalar	SPATMS
DIST3	average wind speed used to develop dispersion equations [m/s]	scalar	SPATMS
EMFRAC	fraction of nuclide released from vegetation in agricultural fires, energy fires, or land and forest fires []	MXCHEM, MXFIRE	SPEMFR
FIRFRQ	frequency of agricultural fires [1/a]	MXBSTA	SPATM2
INDRN	indoor radon transfer coefficient [(mol/m ³)/(mol/kg)]	MXBSTA	SPATM2
INFILT	building infiltration rate [1/s]	scalar	SPATM2
RELFRC	nuclide fraction released from water during indoor usage []	MXCHEM	SPATM2
SOILRN	radon emission source rate [kg/m ² .s]	MXBSTA	SPATM2
WAKE	plume wake entrainment coefficient []	scalar	SPATM2
WIND	average wind speed [m/s]	MXBSTA	SPATM2

Table 6-23: Biosphere Conversion and Yield Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AYIELD	animal food yield [quantity/a]	NANIML	SPAYLD
CRPFRC	fraction of contaminant lost from soil due to cropping that is permanently removed []	scalar	SPCROP
DWS	dry to wet soil mass conversion factor []	scalar	SPFCTR
EPEAT	energy content of peat [MJ/kg]	scalar	SPWLBP
EWOOD	energy content of wood [MJ/kg]	scalar	SPWLBP
FORYP	forest yield [kg/m ²]	scalar	SPWLBP
SBC	soil to inorganic building material mass conversion factor []	scalar	SPFCTR
RENEW	forest renewal time [a]	MXBSTA	SPWLBP
WDW	wet to dry wood mass conversion factor []	scalar	SPFCTR

Table 6-24: Reference Human Group Lifestyle Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CRPFRQ	field cropping frequency [1/a]	MXFELD	SPCROP
CROPER	duration of use of unirrigated field [a]	scalar	SPCROP
DEMMAN	water demand per person [m ³ /a]	MXBSTA	SPWBIO
FUELUS	fuel consumption [MJ/a]	scalar	SPWLBP
LFTIM	household lifetime [a]	MXBSTA	SPWLBP
IRRPER	duration of use of irrigated field [a]	MXBSTA	SPSOIL
NUMMAN	number of persons in household []	MXBSTA	SPWBIO
PRODMD	indicates domestic water source; Lake=1, Well=2	MXBSTA	SPPWEL
PROIRD	indicates if field is irrigated; Not irrigated =0, Irrigated=1 []	MXFELD, MXBSTA	SPPIRR
PROLOC	probability that humans or a crop will be in the path of atmospheric nuclides generated by energy fires ($0 \leq \text{PROLOC} \leq 1$) []	MXBSTA	SPEPRO
PROPT	indicates whether peat will be burned for energy source; No = 0, Yes = 1 []	MXBSTA	SPEPRO

Table 6-25: Human Ingestion/Inhalation Conversion Factor Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CCONT	food carbohydrate content [g/quantity]	MXFOOD, MXBSTA	SPINRT
CFVALU	carbohydrate fuel value [kJ/g]	scalar	SPINRT
DRATE	Man's drinking water rate [L/a]	MXBSTA	SPINRT
ENERGY	Man's total energy need [kJ/d]	scalar	SPINRT
FCONT	food fat content [g/quantity]	MXFOOD, MXBSTA	SPINRT
FFVALU	fat fuel value [kJ/g]	scalar	SPINRT
FRATEI	Man's food ingestion rate input [g/d]	MXFOOD, MXBSTA	SPINRT
IRATE	Man's inhalation rate [m ³ /a]	MXBSTA	SPINRT
PCONT	food protein content [g/quantity]	MXFOOD, MXBSTA	SPINRT
PFVALU	protein fuel value [kJ/g]	scalar	SPINRT
SOILHD	soil ingestion from hands [kg/a]	MXBSTA	SPSING

Table 6-26: Animal Ingestion/Inhalation Conversion Factor Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
ADRINK	animal's drinking water ingestion rate [L/d]	NANIML, MXBSTA	SPDOSA
ATCOEF	fish to water concentration ratio [(mol/kg)/(mol/L)]	MXCHEM	SPDOSA
FEEDR	animal's feed consumption rate [kg/d]	NANIML, MXBSTA	SPDOSA
IRATEA	terrestrial animal's inhalation rate [m ³ /d]	NANIML, MXBSTA	SPDOSA
SOILR	animal's soil ingestion rate [kg/d]	NANIML, MXBSTA	SPDOSA
TACOEf	terrestrial animal air transfer coefficient [(mol/kg or L)/(mol/d)]	MXCHEM, NANIML, MXBSTA	SPDOSA
TCOEfF	terrestrial animal food transfer coefficient [(mol/kg or L)/(mol/d)]	MXCHEM, NANIML, MXBSTA	SPDOSA

Table 6-27: Input Parameters for Determination of Doses from Plants (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CRATIN	ratio of nuclide concentration in wet (fresh) plant matter to that in dry soil for forage field plants []	MXCHEM, MXBSTA	SPCRAT
CRATIO	ratio of nuclide concentration in wet (fresh) plant matter to that in dry soil for garden plants []	MXCHEM, MXBSTA	SPCRAT
DRYDEP	dry deposition velocity [m/s]	MXBSTA	SPDOSP
PHLIFE	plant environment half-life [d]	MXBSTA	SPDOSP
PHLIFF	forage plant environment half-life [d]	MXBSTA	SPDOSP
PHLIFN	plant environment life used in non-human dose calculations [d]	MXBSTA	SPDOSP
PIFRAC	plant interception fraction []	NTERR, NDEPOS, MXBSTA	SPDOSP
PYIELD	plant yield (biomass density) [kg.m-2]	NTERR, MXBSTA	SPPYLD
SOILPT	soil contamination of plants [kg/kg]	scalar	SPSING
TEXPOS	animal's food exposure time [d]	MXTERR, MXBSTA	SPDOSP
WASHOT	washout ratio []	scalar	SPDOSP

Table 6-28: Occupancy Factor Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
BLDOCC	building occupancy factor []	MXBSTA	SPOCPF
GROCC	ground exposure occupancy factor []	MXBSTA	SPOCPF
HALFHI	highest daughter half life [a] Note: Ingrowth in building materials and foods during delay from harvesting is included for shorter lived daughters only.	scalar	SPHLMT
HUMOCC	human occupancy factor []	MXBSTA	SPOCPF
NHMOCC	non-human occupancy factor []	MXBSTA	SPOCPF
TBUILD	exposure to wood building material [d]	scalar	SPDBLG
WIFRAC	plant interception fraction for wood []	scalar	SPDBLG
WOODYD	plant yield for wood [kg/m ²]	scalar	SPDBLG
WTROCC	water immersion occupancy factor []	scalar	SPOCPF

Table 6-29: Holdup Time Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
HAAIR	animal's air inhalation holdup time [d]	NANIML	SPHOLD
HAFOOD	terrestrial animal feed holdup time [d]	NANIML, MXBSTA	SPHOLD
HASOIL	animal's soil ingestion holdup time [d]	NANIML	SPHOLD
HAWATR	animal's drinking water holdup time [d]	NANIML	SPHOLD
HFISH	fish holdup time [d]	MXBSTA	SPHOLD
HINORG	inorganic building material holdup time [d]	MXBSTA	SPHOLD
HMWATR	man's drinking water holdup time [d]	MXBSTA	SPHOLD
HPLANT	plant holdup time [d]	scalar	SPHOLD
HWOOD	wood building material holdup time [d]	MXBSTA	SPHOLD

Table 6-30: Human Dose Coefficient Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
AIRDCF	air immersion dose conversion factor [(Sv/a)/(Bq/m ³)]	MXSPEC	SPAIDC
BLDDCF	building material dose conversion factor [(Sv/a)/(Bq/kg)]	MXSPEC	SPBLDC
GRDCF	ground exposure dose conversion factor [(Sv/a)/(Bq/kg)]	MXSPEC	SPGRDC
IDCF	ingestion dose conversion factor [Sv/Bq] Note: IDCF for I 129 must be set to unity since this dose rate is calculated using INDCF (see Table 6.34).	MXSPEC	SPIDCF
INHDCF	inhalation dose conversion factor [Sv/Bq]	MXSPEC	SPINDC
WTRDCF	water immersion dose conversion factor [(Sv/a)/(Bq/m ³)]	MXSPEC	SPWTDC

Table 6-31: Conversion Factors for Calculating Internal C Dose (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CADCF	internal dose conversion factor for C-14 [(Sv/a)/(Bq/kg)]	scalar	SPCRBN
NHC	carbon concentration in non-human [kg/kg]	MXNHUM	SPCRBN
SCAGW	annual average groundwater concentration of stable carbon [kg/L]	scalar	SPCRBN
SOFCA	carbon content of soft tissue [kg]	scalar	SPCRBN
SOFMAS	mass of soft tissue [kg]	scalar	SPCRBN

Table 6-32: Conversion Factors for Calculating Internal Cl Dose (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CLDCF	internal dose conversion factor for CL-36 [(Sv/a)/(Bq/kg)]	scalar	SPCHLR
NHCL	chlorine concentration in non-human [kg/kg]	MXNHUM	SPCHLR
SCLGW	annual average groundwater concentration of stable chlorine [kg/L]	scalar	SPCHLR
SOFCL	chlorine content of soft tissue [kg]	scalar	SPCHLR

Table 6-33: Conversion Factors for Calculating Tritium Dose (INP File)

Parameter	Definition [Units]	Dimension	Common Block
HDCF	internal dose conversion factor for H-3 [(Sv/a)/(Bq/kg)]	scalar	SPHYD3
HYMAN	hydrogen concentration in man [g/kg]	scalar	SPHYD3
HYWD	hydrogen concentration in wooden building materials [g/kg]	scalar	SPHYD3
HYWTR	hydrogen concentration in water [g/m ³]	scalar	SPHYD3
NHH	tritium concentration in non-human [g/kg]	MXNHUM	SPHYD3

Table 6-34: Conversion Factors for Calculating Internal I Dose (INP File)

Parameter	Definition [Units]	Dimension	Common Block
INDCF	internal dose conversion factor for I-129 for thyroid specific activity model [(Sv/a)/(Bq/kg)]	scalar	SPITHY
NHI	iodine concentration in non-human [kg/kg]	MXNHUM	SPITHY
SINGW	concentration of stable iodine in water [kg/L]	scalar	SPITHY
THYIDN	iodine content of thyroid [kg]	scalar	SPITHY
THYMAS	mass of thyroid [kg]	scalar	SPITHY

Table 6-35: Non-human Dose Conversion Factors (INP File)

Parameter	Definition [Units]	Dimension	Common Block
ANIDCF	animal internal dose conversion factor for I-129 [(Gy/a)/(Bq/kg)]	NHNANI	SPNDCF
NHADCF	non-human air immersion dose conversion factor [(Gy/a)/(Bq/m ³)]	MXSPEC	SPNDCF
NHIDCF	non-human ingestion dose conversion factor [(Gy/a)/(Bq/kg)]	MXSPEC	SPNDCF
NHSDCF	non-human soil immersion dose conversion factor [(Gy/a)/(Bq/kg)]	MXSPEC	SPNDCF
NHVD CF	non-human vegetation immersion dose conversion factor [(Gy/a)/(Bq/kg)]	MXSPEC	SPNDCF
NHWDCF	non-human water immersion dose conversion factor [(Gy/a)/(Bq/m ³)]	MXSPEC	SPNDCF

Table 6-36: Other Input Parameters (INP File)

Parameter	Definition [Units]	Dimension	Common Block
CNLIM	compartment concentration limits [mol/kg]	NCOMP	SPCLIM
CNTIME	user specified time used to calculate consequences [a]	scalar	SPTIME

Table 6-37: Vault Model Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
CAPDZS	damaged zone capacity factor for each vault sector []	MXCHEM,MDPCAPS AXSEC	
CAPRKS	near-field rock capacity factor for each vault sector []	MXCHEM,MDPCAPS AXSEC	
DARBV	Darcy velocity in buffer [m/a]	MAXSEC	DPDARV
DARDZA	axial Darcy velocity in damaged zone [m/a]	MAXSEC	DPDARV
DARDZR	radial Darcy velocity in damaged zone [m/a]	MAXSEC	DPDARV
DARFVA	axial Darcy velocity in backfill [m/a]	MAXSEC	DPDARV
DARFVR	radial Darcy velocity in backfill [m/a]	MAXSEC	DPDARV
DARKVA	Darcy velocity parallel to the axis of the disposal room for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	DPDARV
DARKVR	Darcy velocity orthogonal to the axis of the disposal room for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	DPDARV
DISPRV	longitudinal hydrodynamic dispersion coefficient for element in bottom geosphere segment connected to vault sector [m ² /a]	MXCHEM,MDPDARV AXSEC	
DISTRV	transverse hydrodynamic dispersion coefficient for element in bottom geosphere segment connected to vault sector [m ² /a]	MXCHEM,MDPDARV AXSEC	
FRACU	fraction of used fuel dissolved in one container up to the end of the simulation []	MAXSEC	DPRACU
INVTRY	initial nuclide inventories in vault [mol]	MXSPEC	DPINVT
NCONFS	number of failed containers in each vault sector []	MAXSEC	DPIFRT
PORDZC	porosity in damaged zone []	scalar	DPPORD
TNCONV	total number of containers in the vault []	scalar	DPIFRT
SOLUNX	nuclide solubilities [mol/m ³]	MXSPEC	DPSOLM
SOLUNN	calculated nuclide solubility [mol/m ³]	MXSPEC	DPSOLU
TWSTFM	initial mass of wasteform in vault [kg]	MXMTRX	DPRACU

Table 6-38: Geosphere Network Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
DRAWDN	hydraulic head drawdown [m]	MAXNOD	DPNODS
MNHEAD	modified hydraulic head [m]	MAXNOD	DPNODS
RETGEO	retardation factor []	MXCPCL,MXCHEM	DPRETG
SGGWVH	average linear groundwater velocity [m/a]	MAXSEG	DPSEGS
SGLNTH	segment length [m]	MAXSEG	DPSEGS
SGSFRA	final source fraction []	MAXSEG	DPSEGS

Table 6-39: Discharge and Well Model Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
LASRET	retardation factors for the last geosphere segments leading to a biosphere discharge []	MAXLOC, MXCHEM	DPLSRT
MAREAD	modified discharge area from geosphere [m ²]	MAXLOC	DPVDSC
MVDISC	modified annual discharge volume from geosphere [m ³ /a]	MAXLOC	DPVDSC
OVWDPT	overburden well maximum depth [m]	scalar	DPWELL
QWCAP	volumetric well capacity [m ³ /a]	scalar	DPWELL
QWDEM	volumetric demand on well [m ³ /a]	scalar	DPWELL
QWSUR	surface water flow into well [m ³ /a]	scalar	DPWELL
SEDKD	sediment distribution coeff. [L/kg]	MAXLOC, MXCHEM	DPSDKD
SEDPR	sediment porosity []	MAXLOC	DPSDKD
TPWID	total plume width near well [m]	scalar	DPWELL
WBDISF	well bypass discharge factor []	scalar	DPWELL
WPLMC	well plume capture fraction []	scalar	DPWELL
YGWD	orthogonal distance from central flow line of well to groundwater divide [m]	scalar	DPWELL

Table 6-40: Geosphere/Vault Interface Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
CAPRKV	capacity factor for element in bottom geosphere segment connected to vault sector []	MXCHEM, MAXSEC	PARLGV
DARRK	Darcy velocity for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	PARLGV
DARRKX	Darcy velocity in the x-coordinate direction for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	PARLGV
DARRKY	Darcy velocity in the y-coordinate direction for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	PARLGV
DARRKZ	Darcy velocity in the z-coordinate direction for the bottom geosphere segment connected to vault sector [m/a]	MAXSEC	PARLGV
DSVYRK	dispersion length in the bottom geosphere segment connected to vault sector [m]	MAXSEC	PARLGV
PERMRK	isotropic permeability in the bottom geosphere segment connected to vault sector [m ²]	MAXSEC	PARLGV
PORRK	porosity in the bottom geosphere segment connected to vault sector []	MAXSEC	PARLGV
TORRK	tortuosity in the bottom geosphere segment connected to vault sector []	MAXSEC	PARLGV

Table 6-41: Biosphere Transport Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
AREAF	area of each field [m ²]	MXFELD, MXBSTA	DPANAR
CNGDSR	flag that domestic water source has been changed from "well" to "lake", 0/1 = No/Yes []	MXBSTA	DPWSRC
CNGFSR	flag that field irrigation source has been changed due to use of lake sediment or limited well capacity, 0/1 = No/Yes []	MXFELD, MXBSTA	DPWSRC
NUMANI	number of food animals per household []	NANIML, MXBSTA	DPANAR
PARTIM	particulate deposition time [a]	scalar	DPPRTM

Table 6-42: Biosphere Dose Model Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
CHKCR	check on plant-soil concentration ratio for garden plants []	MXSPEC, MXBSTA	DPCHKR
CHKCRN	check on plant-soil concentration ratio for forage field plants []	MXSPEC, MXBSTA	DPCHKR
FRATE	man's food ingestion rate [kg/a]	MXFOOD, MXBSTA	DPDOSE
LTIM	times used to interpolate time series [a]	NLTIM	DPLTIM
TOTENG	total energy input implied by FRATE [kJ/d]	scalar	DPDOSE

Table 6-43: Irrigation Model Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
IRRIGN	field irrigation source []	MXFELD	DPIRGN
STYPE	index for soil type []	scalar	DPSOLI

Table 6-44: Vault Consequence Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
PRCPMX	maximum amount of precipitate [mol]	MAXSEC MXSPEC	CQVLTO
SECMXT	time of maximum release rate from each vault sector for each nuclide [a]	MAXSEC MXSPEC	CQVLTO
SECMXV	maximum release rate from each vault sector for each nuclide [mol/a]	MAXSEC MXSPEC	CQVLTO
VAREAS	total release from the vault for each vault sector and each nuclide to TLIMIT [mol]	MAXSEC MXSPEC	CQVLTO

Table 6-45: Geosphere Consequence Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
CQGCNT	counter for number of stored consequences [quantity]	scalar	CQLABL
GIFLOW	geosphere integrated flow rate [mol]	MXGCNQ	CQGNET
GMFLOW	geosphere maximum flow rate [mol/a]	MXGCNQ	CQGNET
GTMAXF	geosphere time of maximum flow rate [a]	MXGCNQ	CQGNET
LABEL	label for consequence []. This is a coded value including the NUCPAR (n) and NODE# (p). For NUCPAR<11 - n00ppp For 10 < NUCPAR < 100 - nn0ppp0	MXGCNQ	CQLABL

Table 6-46: Maximum Total Dose to Man

Parameter	Definition [Units]	Dimension	Common Block
MXTDA	maximum total dose rate to man from all nuclides up to a user specified time [Sv/a]	scalar	CQDDA
MXLDA	maximum total dose rate to man from all nuclides up to time TLIMIT [Sv/a]	scalar	CQDDA
TMXTDA	time of maximum total dose rate to man from all nuclides up to a user specified time [a]	scalar	CQDDA
TMXLDA	time of maximum total dose rate to man from all nuclides up to time TLIMIT [a]	scalar	CQDDA
VALDA	value of time series of total dose rate to man from all nuclides at a given time [Sv/a]	NLTIM	CQDDA

Table 6-47: Maximum Nuclide Dose to Man

Parameter	Definition [Units]	Dimension	Common Block
MXTDDT	maximum dose in the DDT times series for each nuclide at TMXTDA years [Sv/a]	MXSPEC	CQMXRN
MXLDT	maximum total dose rate to man from current nuclide up to time TLIMIT [Sv/a]	MXSPEC	CQMXRN
TMXLDT	time of maximum total dose rate to man from current nuclide up to time TLIMIT [a]	MXSPEC	CQMXRN
TPEAK	time of the maximum dose rate of the two highest dose nuclides [a]	MXSPEC	CQPEAK
PEAKDS	dose rate of the two highest dose nuclides for all pathways taken at TPEAK [Sv/a]	MXSPEC, NPATH	CQPEAK

Table 6-48: Integrated Nuclide Dose to Man

Parameter	Definition [Units]	Dimension	Common Block
VALDT	value of total dose rate to man from the current nuclide at a given time [Sv/a]	MXSPEC, NLTIM	CQNH11
CNUCID	nuclide chain number of the highest ranked maximum dose []	MXSPEC	CQNH12

Table 6-49: Maximum Total Dose Rate to Non-Human Biota

Parameter	Definition [Units]	Dimension	Common Block
MXTDNA	maximum total dose rate to non-human biota from all nuclides up to a user specified time [Sv/a]	MXNHUM	CQNHTD
MXLDNA	maximum total dose rate to non-human biota from all nuclides up to time TLIMIT [Sv/a]	MXNHUM	CQNHTD
TMTDNA	time of maximum total dose rate to non-human biota from all nuclides up to a user specified time [a]	MXNHUM	CQNHTD
TMLDNA	time of maximum total dose rate to non-human biota from all nuclides up to time TLIMIT [a]	MXNHUM	CQNHTD
VALDNA	Value of time series of total dose rate to non-human biota from all nuclides at a given time [Sv/a]	NLTIM, MXNHUM	CQNHTD

Table 6-50: Maximum Nuclide Dose Rates to Non-Human Biota

Parameter	Definition [Units]	Dimension	Common Block
PEKDSB	bird dose rate for all pathways taken at time TPEAKB [Sv/a]	MXSPEC, NPATHB	CQPKNH
PEKDSF	fish dose rate for all pathways taken at time TPEAKF [Sv/a]	MXSPEC, NPATHF	CQPKNH
PEKDSP	plant dose rate for all pathways taken at time TPEAKP [Sv/a]	MXSPEC, NPATHP	CQPKNH
PEKDSM	mammal dose rate for all pathways taken at time TPEAKM [Sv/a]	MXSPEC, NPATHM	CQPKNH
MXLDTB	maximum value of the total dose rate to birds from current nuclide up to time TLIMIT [Sv/a]	MXSPEC	CQPKNH
MXLDTF	maximum value of the total dose rate to fish from current nuclide up to time TLIMIT [Sv/a]	MXSPEC	CQPKNH
MXLDTP	maximum value of the total dose rate to plants from current nuclide up to time TLIMIT [Sv/a]	MXSPEC	CQPKNH
MXLDTM	maximum value of the total dose rate to mammals from current nuclide up to time TLIMIT [Sv/a]	MXSPEC	CQPKNH
TPEAKB	time of maximum dose rate to birds [a]	MXSPEC	CQPKNH
TPEAKF	time of maximum dose rate to fish [a]	MXSPEC	CQPKNH
TPEAKP	time of maximum dose rate to plants [a]	MXSPEC	CQPKNH
TPEAKM	time of maximum dose rate to mammals [a]	MXSPEC	CQPKNH
VALDTB	total dose rate to birds from the current nuclide at a given time [Sv/a]	MXSPEC, NLTIM	CQPKNH
VALDTF	total dose rate to fish from the current nuclide at a given time [Sv/a]	MXSPEC, NLTIM	CQPKNH
VALDTP	total dose rate to plants from the current nuclide at a given time [Sv/a]	MXSPEC, NLTIM	CQPKNH
VALDTM	total dose rate to mammals from the current nuclide at a given time [Sv/a]	MXSPEC, NLTIM	CQPKNH

Table 6-51: Concentration and Mass Accumulation Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
MXELCN	maximum element concentration in biosphere compartment [mol/quantity]	MXCHEM, NCCOMP	CQCOMP
TMXELC	time of maximum element concentration in biosphere compartment [a]	MXCHEM, NCCOMP	CQCOMP
MXGFLX	maximum value of the time series for the total radiotoxicity flux for all nuclides from the geosphere to the biosphere up to time TLIMIT [Sv/a]	scalar	CQSFIN
TMXGFL	time of maximum value of the time series for the total radiotoxicity flux for all nuclides from the geosphere to the biosphere up to time TLIMIT [a]	scalar	CQSFIN
MXLAKE	maximum value of the time series for the total radiotoxicity concentration for all nuclides in lake water up to time TLIMIT [Sv/m3]	scalar	CQSFIN
TMXLAK	time of maximum value of the time series for the total radiotoxicity concentration for all nuclides in lake water up to time TLIMIT [a]	scalar	CQSFIN
MXLCN	maximum concentration of the current biosphere compartment up to TLIMIT [mol/kg]	MXSPEC, NCOMP	CQCOMP
TMXLCN	time of maximum concentration of the current biosphere compartment up to TLIMIT [mol/kg]	MXSPEC, NCOMP	CQCOMP
MTLSL	total mass of nuclide in lake sediment at TLIMIT years [mol]	MXSPEC	CQMASS
MTLWL	total mass of nuclide in lakewater at TLIMIT years [mol]	MXSPEC	CQMASS
MTSL	total mass of nuclide in soil at TLIMIT years [mol]	MXSPEC, MXFELD	CQMASS

Table 6-52: Maximum Activity in Food-chain Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
MXLAA	maximum concentration/activity in animal due to contamination in air up to TLIMIT years [quantity]	NANIML, MXSPEC	CQCHN1
MXLAL	maximum concentration/activity in animal due to contamination in leaves up to TLIMIT years [quantity]	NANIML, MXSPEC	CQCHN1
MXLAR	maximum concentration/activity in animal due to contamination in roots up to TLIMIT years [quantity]	NANIML, MXSPEC	CQCHN1
MXLAS	maximum concentration/activity in animal due to contamination in soil up to TLIMIT years [quantity]	NANIML, MXSPEC	CQCHN1
MXLAW	maximum concentration/activity in animal due to contamination in water up to TLIMIT years [quantity]	NANIML, MXSPEC	CQCHN1
MXLF	maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated fish up to TLIMIT years [quantity]	MXSPEC	CQCHN1
MXLPL	maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated leaves up to TLIMIT years [quantity]	MXSPEC	CQCHN1
MXLPR	maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated roots up to TLIMIT years [quantity]	MXSPEC	CQCHN1
TMXLAA	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide of consumed animal due to contamination in air up to TLIMIT years [a]	NANIML, MXSPEC	CQCHN2
TMXLAL	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide of consumed animal due to contamination in leaves up to TLIMIT years [a]	NANIML, MXSPEC	CQCHN2

Table 6-53: Maximum Activity in Food-chain Output Parameters (concluded)

Parameter	Definition [Units]	Dimension	Common Block
TMXLAR	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide of consumed animal due to contamination in roots up to TLIMIT years [a]	NANIML, MXSPEC	CQCHN2
TMXLAS	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide of consumed animal due to contamination in soil up to TLIMIT years [a]	NANIML, MXSPEC	CQCHN2
TMXLAW	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide of consumed animal due to contamination in water up to TLIMIT years [a]	NANIML, MXSPEC	CQCHN2
TMXLF	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated fish up to TLIMIT years [a]	MXSPEC	CQCHN2
TMXLPL	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated leaves up to TLIMIT years [a]	MXSPEC	CQCHN2
TMXLPR	time of maximum concentration/activity of a toxic, non-radionuclide/radionuclide consumed due to contaminated roots up to TLIMIT years [a]	MXSPEC	CQCHN2
RNTOX	index to indicate radionuclide or toxic, non-radionuclide []	MXSPEC	CQCHNI

Table 6-54: Biosphere Water Source Output Parameters

Parameter	Definition [Units]	Dimension	Common Block
DMST	index used to identify domestic source of water []	MXBSTA	CQWSRC
FORG	index used to identify field type []	MXBSTA	CQWSRC
PTBG	index used to identify the peatbog []	MXBSTA	CQWSRC
VEGE	index used to identify the vegetable patch []	MXBSTA	CQWSRC
WDLT	index used to identify the woodlot []	MXBSTA	CQWSRC

Table 6-55: Biosphere Warning Output Parameters

Parameter	Definition [Units]	Dimension*	Common Block
WCNLIM	warning flag indicating peak compartment concentration MXLCN is greater than the maximum allowed limit CNLIM []	MXSPEC, NCOMP	CQWARN
WGWDLM	warning flag indicating total internal dose for nuclide has been lowered to the groundwater dilution limit GWDLMT for at least one time point []	MXGDLN	CQWARN
WGWDNH	warning flag indicating total non-human biota internal dose for nuclide has been lowered to the groundwater dilution limit GWDLMT for at least one time point []	MXNHUM, MXGDLN	CQWARN
WMVDSC	warning flag indicating modified discharge volume is less than the modified discharge volume limit, MVDSC, and has been set to zero []	MAXLOC	CQWARN
TGWDLM	time at which pathway doses become meaningless because groundwater dilution limit was exceeded [a]	MXGDLN	CQWRN2
TGWDNH	time at which pathway doses become meaningless for non-human biota because groundwater dilution limit was exceeded [a]	MXNHUM, MXGDLN	CQWRN2

* Dimension of MXGDLN accounts for C-14, Cl-36 and I-129 in Fuel and Zircaloy.

Table 6-56: Mass Accumulation and Distribution Parameters

Parameter	Definition [Units]	Dimension	Common Block
AMTBIO	Amount accumulated in biosphere [mol]	MXSPEC	CQBIOA
AMTCNT	Amount accumulated in failed containers [mol]	MXSPEC	CQCNTA
AMTDSR	Amount accumulated in downstream release [mol]	MXSPEC	CQBIOA
AMTGEO	Amount accumulated in geosphere [mol]	MXSPEC	CQGEOA
ATICNT	Amount accumulated in intact containers [mol]	MXSPEC	CQCNTA
AMTVLT	Amount accumulated in vault sealing materials and EDZ [mol]	MXSPEC	CQVLTA
DCYBIO	Amount decayed in biosphere [mol]	MXSPEC	CQBIOA
DCYCNT	Amount decayed in failed containers [mol]	MXSPEC	CQCNTA
DCYDSR	Amount decayed in downstream release [mol]	MXSPEC	CQBIOA
DCYGEO	Amount decayed in geosphere [mol]	MXSPEC	CQGEOA
DCICNT	Amount decayed in intact containers [mol]	MXSPEC	CQCNTA
DCYVLT	Amount decayed in vault sealing materials and EDZ [mol]	MXSPEC	CQVLTA
INFBIO	amount released into biosphere [mol]	MXSPEC	CQBIOA
INGRBT	Ingrowth from parent in biosphere [mol]	MXSPEC	CQBIOA
INGRCT	Ingrowth from parent in failed containers [mol]	MXSPEC	CQCNTA
INGRDS	Ingrowth from parent in downstream release [mol]	MXSPEC	CQBIOA
INGRGT	Ingrowth from parent in geosphere [mol]	MXSPEC	CQGEOA
INGICT	Ingrowth from parent in intact containers [mol]	MXSPEC	CQCNTA
INGRVT	Ingrowth from parent in vault sealing materials and EDZ [mol]	MXSPEC	CQVLTA
MBRBIO	mass balance ratio for biosphere []	MXSPEC	CQBIOA
RELBIO	Amount released from biosphere [mol]	MXSPEC	CQBIOA
RELCNT	Amount released from failed containers [mol]	MXSPEC	CQCNTA
RELDNR	Amount released from downstream [mol]	MXSPEC	CQBIOA
RELGEO	Amount released from geosphere [mol]	MXSPEC	CQGEOA
RLICNT	Amount released from intact containers [mol]	MXSPEC	CQCNTA
RELVLT	Amount released from vault sealing materials and EDZ [mol]	MXSPEC	CQVLTA

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APPENDIX A: EXAMPLE SIMULATION COMMAND FILE

The following command file copies in the required INCLUDE files from a directory \inc\ that contains all the SP*.INC, DP*.INC, and CQ*.INC files, into the current directory which contains the main input file, (SV01.INP), any FXD files and optionally any FRAC3DVS data files. Then it submits the simulation with the appropriate prompts, deletes copied INCLUDE files, and renames the new output files. Although not explicitly listed here, the full set of input files could include SV01.INP, SOLSV01.FXD, NETSV01.FXD, SORSV01.FXD, F3DSV01.FXD and MDNAA10.QNT.

Contents of Command File

```
copy ..\inc\*.INC *.*
pause
..\..\..\release\SCC408 <prompt.dat >SV_01.log
pause
del *.inp
rename SV100101.DOS SV_01.DOS
rename SV100101.SUB SV_01.GEO
rename SV100101.CDS SV_01.VLT
rename SV100101.NDS SV_01.BIO
rename SV100101.LPT SV_01.LPT
rename SV100101.PAR SV_01.PAR
rename SV100101.OUT SV_01.OUT
```

Contents of Prompt.Dat file

```
SV01
N
```


APPENDIX B: LAYOUT OF SYVAC3-CC4 MAIN INPUT FILE

Below is an extraction from the SYVAC_MEDIAN.IHB input file median case simulation. The input file was generated from the Fourth Case Study database 2011_01. Only the general format of the input file is included in this document, as the entire input file would run to hundreds of pages.

Main Input File

```
! Input file generated by/singen3 2/int:/RepositorySafety/FourthCaseStudy/4CS.../
! Fri Jul 29 13:26:05 2011      VERSION 01A
! Group HB
! Derived from database: database/SCC408/2011_01
!
! Case title:
'Median - SCC408'
!
! Output type ( choose 'LONG' or 'SHORT' ):
'LONG'
!
! Optional outputs:
'PAR' ! for all parameter values
& 'SUB' ! for time series during geosphere execution
& 'NDS' ! for time series during biosphere execution
& 'CDS' ! for time series during vault execution
!
! Number of simulations for this case:
1 1 1 ! range 1: start #requested end (integers)
! Insert more lines for more (non-overlapping) ranges
!
! Time series control:
1.0D1 1.8D1 3.2D1 5.6D1 1.0D2 1.8D2
& 3.2D2 5.6D2 1.0D3 1.8D3 3.2D3 5.6D3
& 1.0D4 1.8D4 3.2D4 5.6D4 1.0D5 1.8D5
& 3.2D5 5.6D5 1.0D6 1.8D6 3.2D6 5.6D6
& 1.0D7 ! Fixed times (years) (d.p.)
3 200 ! Minimum and maximum number of time steps (integers)
& 0.001 ! Target fractional error for time series representation (d.p. 0 to 1)
& 0.2 0.2 ! time series smoothing controls! VLT include files:
'CQCNTA.INC'...
'SPVLT.INC'
! GEO include files:
'CQGEOA.INC'...
'SPWELL.INC'
! BIO include files:
'CQBIOA.INC'...
'SPWTDC.INC'
'END' ! end of INCLUDE file list
!
! Parameters are grouped by model in the order VLT GEO BIO.
! Within each model, parameters are grouped by type in the order
! SP DP CQ. There are two SP groups for each model,
! nuclide independent and nuclide dependent.
! Within each group, parameters are sorted alphabetically
! (with the exception of correlated parameters and grouped parameters)
!
! Nuclide Independent Parameters
!
'QUANTILE' 'MEDIANHB.QNT'
!
! VLT SPALPH.INC COMMON/SPALPH/ AALPHA
'ALPHA DOSE DISS. RATE EXPONENT ' 'AALPHA ' 'S'
& 'CONST' 1.0 !K. WEI
...
```

```

!                                     !FRANK GARISTO
!INSTANT RELEASE FRAC. DUM17      ' 'IRFRAV(040)      ' '[]      ' 'N'
& 'CONST' 0.0                                !A. D'ANDREA
!
! GEO  SPSTAT.INC  COMMON/SPSTAT/  TDURAT(MAXPER)
!GLACIAL PERIOD DURATION  GP001'  'TDURAT(001)      ' '[A]      ' 'S'
& 'CONST' 50300
...
!GLACIAL PERIOD DURATION  GP100'  'TDURAT(100)      ' '[A]      !T.CHSHYOLKOVA
& 'CONST' 0                                ' 'S'
!T.CHSHYOLKOVA
!END'      ! END OF ALL SAMPLED PARAMETERS
!
!CALCULATED'
!
! Nuclide Independent Parameters
!
! VLT  DPDARV.INC  COMMON/DPDARV/  DARBV(MAXSEC)
!SECTOR BUFFER DARCY VEL.  sec01'  'DARBV(01)      ' '[M/A]      ' 'S' 1
...
!NUCLIDE SOLUBILITIES      dum17'  'SOLUNX(040)      ' '[MOL/M3]      ' 'N' 1
!END'      ! end of DP parameters for VLT
!
!CALCULATED'
!
! Nuclide Independent Parameters
!
! GEO  DPNODS.INC  COMMON/DPNODS/  DRAWDN(MAXNOD)
!HYDRAULIC HEAD DRAWDOWN  nd001'  'DRAWDN(001)      ' '[M]      ' 'S' 1
...
!RETARDATION FACTOR  null  dume7'  'RETGEO(10,25)      ' '[]      ' 'N' 1
!END'      ! end of DP parameters for GEO
!
!CALCULATED'
!
! Nuclide Independent Parameters
!
! BIO  DPANAR.INC  COMMON/DPANAR/  AREAOF(MXFELD)
!AREA OF EACH FIELD      forag'  'AREAOF(01)      ' '[M2]      ' 'S' 1
...
!SEDIM" T DIST. COEFF  dis10 dume7'  'SEDKD(10,25)      ' '[L/KG]      ' 'N' 1
!END'      ! end of DP parameters for BIO
!
!CONSEQUENCES'
!
! Nuclide Independent Parameters
!
! Nuclide Dependent Parameters
!
! VLT  CQCNTA.INC  COMMON/CQCNTA/  AMTCNT(MXSPEC)
!AMT ACCUM. IN FAILED CONT. Ac225'  'AMTCNT(001)      ' '[MOL]      ' 'S' 1
& 'NUM' '-1.0'
...
!TOT RELEASE FROM VLT endf1 dum17'  'VAREAS(25,040)      ' '[MOL]      ' 'N' 1
& 'NUM' '-1.0'
!END'      ! end of CQ parameters for VLT
!
!CONSEQUENCES'
!
! Nuclide Independent Parameters
!
! GEO  CQNET.INC  COMMON/CQLABL/  CQGCNT
!STORED CONSEQUENCES COUNTER      ' 'CQGCNT      ' '[QUANTITY]      ' 'S' 1
& 'INT' '-1'
...
!AMT RELEASED FROM GEO      dum17'  'RELGEO(040)      ' '[MOL]      ' 'N' 1
& 'NUM' '-1.0'
!END'      ! end of CQ parameters for GEO

```



```

!
'CONSEQUENCES'
!
!   Nuclide Independent Parameters
!
!   BIO   CQWSRC.INC   COMMON/CQWSRC/   CNGDSR
'WARN: "WELL" CHANGED TO "LAKE"   '   'CNGDSR           '   '[]           '   'S'   1
&   'INT'   '-1'
...
'WARN: SOIL REGR. MODEL           dum17'   'WREGTM(040)           '   '[]           '   'N'   1
&   'INT'   '-1'
!
'END'           ! end of CQ parameters for BIO
'END'           ! end of all parameter descriptions
!
!   start of nuclide chains       NUCLIDE GROUP GTC
'PU241AFUEL'   'AM241AFUEL'   'NP237AFUEL'   '=PA233AFUEL'   'U 233AFUEL'
&   'TH229AFUEL'   '=RA225AFUEL'   '=AC225AFUEL'
'U 238AFUEL'   ! '=TH234AFUEL'   'U 234AFUEL'   'TH230AFUEL'   'RA226AFUEL'
&   '=RN222AFUEL'   '=PB210AFUEL'   '=BI210AFUEL'   '=PO210AFUEL'
'C 14 FUEL'
'CA 41 FUEL'
'CL 36 FUEL'
'TC 99 FUEL'
'SE 79 FUEL'
'I 129 FUEL'
'END'           ! end of nuclide chains
!...start of matrix materials
'U 238AFUEL'
'END'           ! end of matrix materials
!

```


APPENDIX C: EXAMPLE SYVAC3-CC4 MEDIAN CASE SAMPLE FILE

This appendix is an extraction from the HBC median case sample file. This extraction shows the general format of a sample file. In a sample file, all the values needed for a single simulation must appear in a single logical record and there must be as many records as simulations. These files are read as Standard ASCII Files, and so comments and continuation lines are permitted. In this extraction the first few records are displayed, then the quantiles for IFAILQ (the only sampled parameter with quantile values not set to 0.50), and finally the last few records of the quantile file.

Median Case Quantile File

```
!
! Fri Jul 29 13:26:05 2011
!
!!QUANTILE file created from SYVAC_MEDIAN.IHB
! created by SINGEN at /ipa/dev/singen3_2/
! in session T:/RepositorySafety/FourthCaseStudy/4CSDeterministicRuns/
! with default name AUXFILE_1.AUX
!
0.5 !'ALPHA DOSE DISS. RATE EXPONENT ' 'AALPHA ' '[] '
&0.5 !'BETA DOSE DISS. RATE EXPONENT ' 'ABETA ' '[] '
&0.5 !'GAMMA DOSE DISS. RATE EXPONENT ' 'AGAMMA ' '[] '
&0.5 !'ALPHA FUEL DOSE VARY FACTOR ' 'ALFCOF ' '[] '
&0.5 !'FUEL ALPHA DOSE RATES DAT01' 'ALPHDO(01) ' '[GY/A] '
&0.5 !'FUEL ALPHA DOSE RATES DAT02' 'ALPHDO(02) ' '[GY/A] '
&0.5 !'FUEL ALPHA DOSE RATES DAT03' 'ALPHDO(03) ' '[GY/A] '
&0.5 !'FUEL ALPHA DOSE RATES DAT04' 'ALPHDO(04) ' '[GY/A] '
&...
&0.5 !'GAMMA BUNDLE-CONTAINER FACTOR ' 'GAMCOF ' '[] '
&0.5 !'Geff VALUE FOR ALPHA RADIATION ' 'GeffA ' '[MOL.M-2.GY-'
&0.5 !'Geff VALUE FOR BETA AND GAMMA ' 'GeffBG ' '[MOL.M-2.GY-'
&0.903 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC01' 'IFAILQ(01) ' '[] '
&0.911 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC02' 'IFAILQ(02) ' '[] '
&0.916 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC03' 'IFAILQ(03) ' '[] '
&0.911 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC04' 'IFAILQ(04) ' '[] '
&0.897 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC05' 'IFAILQ(05) ' '[] '
&0.872 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC06' 'IFAILQ(06) ' '[] '
&0.886 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC07' 'IFAILQ(07) ' '[] '
&0.893 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC08' 'IFAILQ(08) ' '[] '
&0.893 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC09' 'IFAILQ(09) ' '[] '
&0.905 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC10' 'IFAILQ(10) ' '[] '
&0.915 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC11' 'IFAILQ(11) ' '[] '
&0.903 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC12' 'IFAILQ(12) ' '[] '
&0.903 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC13' 'IFAILQ(13) ' '[] '
&0.889 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC14' 'IFAILQ(14) ' '[] '
&0.893 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC15' 'IFAILQ(15) ' '[] '
&0.853 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC16' 'IFAILQ(16) ' '[] '
&0.861 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC17' 'IFAILQ(17) ' '[] '
&0.924 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC18' 'IFAILQ(18) ' '[] '
&0.913 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC19' 'IFAILQ(19) ' '[] '
&0.918 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC20' 'IFAILQ(20) ' '[] '
&0.896 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC21' 'IFAILQ(21) ' '[] '
&0.903 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC22' 'IFAILQ(22) ' '[] '
&0.900 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC23' 'IFAILQ(23) ' '[] '
&0.977 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC24' 'IFAILQ(24) ' '[] '
&0.955 !0.5 !'INSTANT CONT. FAIL. QUANT. SEC25' 'IFAILQ(25) ' '[] '
&0.5 !'INSTANT FAILURE FRACTION ' 'IFRACT ' '[] '
&...
&0.5 !'INVENTORY, V DUMN1 ' 'INVPKG(040) ' '[MOL/KG] '
&0.5 !'INSTANT RELEASE FRAC. DUMN1 ' 'IRFRAV(040) ' '[] '

```


APPENDIX D: NUCLIDE SOLUBILITY INPUT DATA FILE

This appendix is an extraction from the 4CS element solubility file. In order to minimize the size of this document the uranium information has been show in full but all other elements have been removed.

```
3.0E-02 ! IR1 first reference ionic strength
& 8.0E-01 ! IR2 second reference ionic strength
& 0.0 ! P4(01,01) carbonate index Uranium ! UO2+2
& 0.0 ! P4(01,02) carbonate index Uranium ! UO2+
& 0.0 ! P4(01,03) carbonate index Uranium ! UO2(OH)+
& 0.0 ! P4(01,04) carbonate index Uranium ! (UO2)3(OH)7-
& 0.0 ! P4(01,05) carbonate index Uranium ! UO2(OH)2(AQ)
& 0.0 ! P4(01,06) carbonate index Uranium ! UO2(OH)4-2
& 0.0 ! P4(01,07) carbonate index Uranium ! U(OH)4(AQ)
& 0.0 ! P4(01,08) carbonate index Uranium ! U(OH)5-
& 0.0 ! P4(01,09) carbonate index Uranium ! UO2CL+
& 0.0 ! P4(01,10) carbonate index Uranium ! UO2F+
& 0.0 ! P4(01,11) carbonate index Uranium ! UO2F2(AQ)
& 0.0 ! P4(01,12) carbonate index Uranium ! UO2F3-
& 0.0 ! P4(01,13) carbonate index Uranium ! UO2F4-2
& 0.0 ! P4(01,14) carbonate index Uranium ! UF3+
& 0.0 ! P4(01,15) carbonate index Uranium ! UF4(AQ)
& 1 ! P4(01,16) carbonate index Uranium ! UO2CO3(AQ)
& 2 ! P4(01,17) carbonate index Uranium ! UO2(CO3)2-2
& 6 ! P4(01,18) carbonate index Uranium ! (UO2)3(CO3)6-6
& 3 ! P4(01,19) carbonate index Uranium ! UO2(CO3)3-4
& 5 ! P4(01,20) carbonate index Uranium ! U(CO3)5-6
& 0.0 ! P4(01,21) carbonate index Uranium ! UO2SO4(AQ)
& 0.0 ! P4(01,22) carbonate index Uranium ! UO2(SO4)2-2
& 0.0 ! P4(01,23) carbonate index Uranium ! UO2HPO4(AQ)
& 0.0 ! P4(01,24) carbonate index Uranium ! UO2PO4-
& 0.0 ! P4(02,01) carbonate index Thorium ! ThOH+3
& 0.0 ! P4(02,02) carbonate index Thorium ! Th(OH)2+2
& 0.0 ! P4(02,03) carbonate index Thorium ! Th(OH)3+
& 0.0 ! P4(02,04) carbonate index Thorium ! Th(OH)4(aq)
& 0.0 ! P4(02,05) carbonate index Thorium ! ThF3+
& 0.0 ! P4(02,06) carbonate index Thorium ! ThF4(aq)
& 0.0 ! P4(02,07) carbonate index Thorium ! Th(SO4)2(aq)
& 0.0 ! P4(02,08) carbonate index Thorium ! Th(HPO4)2(aq)
& 0.0 ! P4(02,09) carbonate index Thorium ! Th(HPO4)3-2
& 5 ! P4(02,10) carbonate index Thorium ! Th(CO3)5-6
& 0.0 ! P4(03,01) carbonate index Technetium TcO4-
& 0.0 ! P4(03,02) carbonate index Technetium TcO(OH)+
& 0.0 ! P4(03,03) carbonate index Technetium TcO(OH)2
& 0.0 ! P4(03,04) carbonate index Technetium TcO(OH)3-
& 1 ! P4(03,05) carbonate index Technetium Tc(OH)2CO3(aq)
& 1 ! P4(03,06) carbonate index Technetium Tc(OH)3CO3-
& 0.0 ! P4(04,01) carbonate index Plutonium Pu+3
& 0.0 ! P4(04,02) carbonate index Plutonium PuOH+2
& 0.0 ! P4(04,03) carbonate index Plutonium Pu(OH)4(aq)
& 0.0 ! P4(04,04) carbonate index Plutonium Pu(H2PO4)+2
& 0.0 ! P4(04,05) carbonate index Plutonium PuSO4+
& 0.0 ! P4(05,01) carbonate index Neptunium Np+3
& 0.0 ! P4(05,02) carbonate index Neptunium NpO2+
& 0.0 ! P4(05,03) carbonate index Neptunium Np(OH)2+2
& 0.0 ! P4(05,04) carbonate index Neptunium Np(OH)4(aq)
& 0.0 ! P4(05,05) carbonate index Neptunium NpO2(OH)2-
& 0.0 ! P4(05,06) carbonate index Neptunium NpO2(OH)(aq)
& 0.0 ! P4(05,07) carbonate index Neptunium NpF2+2
& 0.0 ! P4(05,08) carbonate index Neptunium NpO2F(aq)
& 0.0 ! P4(05,09) carbonate index Neptunium Np(SO4)2(aq)
& 0.0 ! P4(05,10) carbonate index Neptunium NpO2SO4-
& 1 ! P4(05,11) carbonate index Neptunium NpO2CO3-
```

```

& 2 ! P4(05,12) carbonate index Neptunium NpO2(CO3)2-3
& 3 ! P4(05,13) carbonate index Neptunium NpO2(CO3)3-5
& 0.0 ! P4(05,14) carbonate index Neptunium NpO2(HPO4)-
& 0.0 ! P4(05,15) carbonate index Neptunium NpO2Cl(aq)
& 0.0 ! P5(01,01) HPO4-2 index Uranium ! UO2+2
& 0.0 ! P5(01,02) HPO4-2 index Uranium ! UO2+
& 0.0 ! P5(01,03) HPO4-2 index Uranium ! UO2(OH)+
& 0.0 ! P5(01,04) HPO4-2 index Uranium ! (UO2)3(OH)7-
& 0.0 ! P5(01,05) HPO4-2 index Uranium ! UO2(OH)2(AQ)
& 0.0 ! P5(01,06) HPO4-2 index Uranium ! UO2(OH)4-2
& 0.0 ! P5(01,07) HPO4-2 index Uranium ! U(OH)4(AQ)
...
& 1 ! MNUM(01,15) number metal atoms Uranium ! UF4(aq)
& 1 ! MNUM(01,16) number metal atoms Uranium ! UO2CO3(aq)
& 1 ! MNUM(01,17) number metal atoms Uranium ! UO2(CO3)2-2
& 3 ! MNUM(01,18) number metal atoms Uranium ! (UO2)3(CO3)6-6
& 1 ! MNUM(01,19) number metal atoms Uranium ! UO2(CO3)3-4
& 1 ! MNUM(01,20) number metal atoms Uranium ! U(CO3)5-6
& 1 ! MNUM(01,21) number metal atoms Uranium ! UO2SO4(aq)
& 1 ! MNUM(01,22) number metal atoms Uranium ! UO2(SO4)2-2
& 1 ! MNUM(01,23) number metal atoms Uranium ! UO2HPO4(aq)
& 1 ! MNUM(01,24) number metal atoms Uranium ! UO2PO4-
& 1 ! MNUM(02,01) number metal atoms Thorium ! ThOH+3
& 1 ! MNUM(02,02) number metal atoms Thorium ! Th(OH)2+2
& 1 ! MNUM(02,03) number metal atoms Thorium ! Th(OH)3+
& 1 ! MNUM(02,04) number metal atoms Thorium ! Th(OH)4(aq)
& 1 ! MNUM(02,05) number metal atoms Thorium ! ThF3+
& 1 ! MNUM(02,06) number metal atoms Thorium ! ThF4(aq)
& 1 ! MNUM(02,07) number metal atoms Thorium ! Th(SO4)2(aq)
& 1 ! MNUM(02,08) number metal atoms Thorium ! Th(HPO4)2(aq)
& 1 ! MNUM(02,09) number metal atoms Thorium ! Th(HPO4)3-2
& 1 ! MNUM(02,10) number metal atoms Thorium ! Th(CO3)5-6
& 1 ! MNUM(03,01) number metal atoms Technetium TcO4-
& 1 ! MNUM(03,02) number metal atoms Technetium TcO(OH)+
& 1 ! MNUM(03,03) number metal atoms Technetium TcO(OH)2
& 1 ! MNUM(03,04) number metal atoms Technetium TcO(OH)3-
& 1 ! MNUM(03,05) number metal atoms Technetium Tc(OH)2CO3(aq)
& 1 ! MNUM(03,06) number metal atoms Technetium Tc(OH)3CO3-
& 1 ! MNUM(04,01) number metal atoms Plutonium Pu+3
& 1 ! MNUM(04,02) number metal atoms Plutonium PuOH+2
& 1 ! MNUM(04,03) number metal atoms Plutonium Pu(OH)4(aq)
& 1 ! MNUM(04,04) number metal atoms Plutonium Pu(H2PO4)+2
& 1 ! MNUM(04,05) number metal atoms Plutonium PuSO4+
& 1 ! MNUM(05,01) number metal atoms Neptunium Np+3
& 1 ! MNUM(05,02) number metal atoms Neptunium NpO2+
& 1 ! MNUM(05,03) number metal atoms Neptunium Np(OH)2+2
& 1 ! MNUM(05,04) number metal atoms Neptunium Np(OH)4(aq)
& 1 ! MNUM(05,05) number metal atoms Neptunium NpO2(OH)2-
& 1 ! MNUM(05,06) number metal atoms Neptunium NpO2(OH)(aq)
& 1 ! MNUM(05,07) number metal atoms Neptunium NpF2+2
& 1 ! MNUM(05,08) number metal atoms Neptunium NpO2F(aq)
& 1 ! MNUM(05,09) number metal atoms Neptunium Np(SO4)2(aq)
& 1 ! MNUM(05,10) number metal atoms Neptunium NpO2SO4-
& 1 ! MNUM(05,11) number metal atoms Neptunium NpO2CO3-
& 1 ! MNUM(05,12) number metal atoms Neptunium NpO2(CO3)2-3
& 1 ! MNUM(05,13) number metal atoms Neptunium NpO2(CO3)3-5
& 1 ! MNUM(05,14) number metal atoms Neptunium NpO2(HPO4)-
& 1 ! MNUM(05,15) number metal atoms Neptunium NpO2Cl(aq)

```

APPENDIX E: GEOSPHERE NETWORK INPUT DATA FILE

This appendix contains the entire 4CS geosphere network input file. The order of node calculations is automatically determined based on segment inlet and outlet information from this file.

```
! 2011-FEB-09  VERSION 03A.01  C. Kitson
!               new network file for 4CS
! Generated in 4CSNetFileConnectivity02a.xls in
! W:\~\SA05_2010\~\03M\03_Sectorization\06_NodeSelection\03_Network
! GEONET - NETWORK FIXED PARAMETER DATA FILE 'NETnn.FXD'
! INPUT FILE FOR SYVAC3-CC407
!               Dimensions of 25 sectors (50 source nodes)
!                   200 nodes
!                   200 segments
!                   10 discharges
!                   10 unique glaciation states
! groundwater velocity function indicator []
!   1 = velocity input
!   2 = darcy velocity input
!   3 = hydraulic conductivity and head input and
!       velocity calculated
!   4 = permeability and head input
!       both hydraulic conductivity and
!       velocity calculated from reference water properties
!   5 = permeability and temperature and head input
!       both hydraulic conductivity and
!       velocity calculated from variable water properties
!   6 = permeability and temperature and head input
!       both hydraulic conductivity and
!       velocity calculated from variable water properties
!       with gravitational buoyancy term
3
&! geosphere fixed parameters for segments
&!response function flags []
&!1 =RSMINF, semi-infinite b.c. response function
&!2 =RMSTFR, mass transfer b.c. response function
&!3 =RZROCO, zero concentration b.c. response function
&!4 =pass without change, no response function
&!5 =MULTIC, compartment model mimic a semi-infinite b.c.
&!6 =MULTIC, compartment model mimic a zero concentration b.c.
&  1  1  1  1  1  1  1  1  4  1  !10
&  1  1  1  1  1  1  1  1  1  1  !20
&  1  1  1  4  1  1  1  1  4  1  !30
&  1  1  1  4  1  1  4  1  1  1  !40
&  1  4  1  1  1  1  1  1  1  4  !50
&  1  1  4  1  1  1  1  1  1  1  !60
&  1  1  4  1  1  4  1  1  1  1  !70
&  1  1  1  1  1  1  1  1  1  4  !80
&  1  1  4  1  1  1  1  1  1  1  !90
&  1  4  1  1  4  1  1  4  1  1  !100
&  1  1  1  1  1  1  1  1  1  1  !110
&  1  1  4  1  1  1  4  1  1  1  !120
&  1  1  1  1  1  1  1  1  4  1  !130
&  1  1  1  1  1  1  1  1  1  4  !140
&  4  1  1  1  1  1  1  1  1  1  !150
&  1  1  1  4  4  4  4  4  4  4  !160
&  4  4  0  0  0  0  0  0  0  0  !170
&  0  0  0  0  0  0  0  0  0  0  !180
&  0  0  0  0  0  0  0  0  0  0  !190
&  0  0  0  0  0  0  0  0  0  0  !200
&! chemical property class
&  2  2  2  4  6  5  5  5  20  2  !10
```

```
& 3 2 2 2 4 2 3 2 2 2 !20
& 4 2 3 20 2 2 2 20 2 2 !30
& 16 10 2 20 2 3 20 2 2 2 !40
& 2 20 2 2 10 16 9 16 10 20 !50
& 2 3 20 2 10 16 2 2 16 9 !60
& 16 10 20 2 2 20 2 3 2 2 !70
& 10 2 2 10 16 9 16 10 2 20 !80
& 2 3 20 2 4 5 2 2 10 2 !90
& 4 20 2 3 20 2 3 20 2 9 !100
& 10 2 10 16 9 16 10 2 16 9 !110
& 16 10 20 2 4 5 20 2 10 16 !120
& 10 16 2 2 4 4 6 20 10 2 !130
& 15 14 15 2 4 2 4 4 6 20 !140
& 20 3 7 8 3 7 8 5 7 8 !150
& 5 7 8 20 20 20 20 20 20 !160
& 20 20 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&! physical property class
& 2 2 2 4 6 5 5 5 20 2 !10
& 3 2 2 2 4 2 3 2 2 2 !20
& 4 2 3 20 2 2 2 20 2 2 !30
& 16 10 2 20 2 3 20 2 2 2 !40
& 2 20 2 2 10 16 9 16 10 20 !50
& 2 3 20 2 10 16 2 2 16 9 !60
& 16 10 20 2 2 20 2 3 2 2 !70
& 10 2 2 10 16 9 16 10 2 20 !80
& 2 3 20 2 4 5 2 2 10 2 !90
& 4 20 2 3 20 2 3 20 2 9 !100
& 10 2 10 16 9 16 10 2 16 9 !110
& 16 10 20 2 4 5 20 2 10 16 !120
& 10 16 2 2 4 4 6 20 10 2 !130
& 15 14 15 2 4 2 4 4 6 20 !140
& 20 3 7 8 3 7 8 5 7 8 !150
& 5 7 8 20 20 20 20 20 20 !160
& 20 20 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!node index number for node at inlet of segment
& 1 2 3 4 5 6 134 135 6 144 !10
& 8 10 11 12 13 145 14 15 16 17 !20
& 18 146 19 20 21 22 23 24 22 25 !30
& 26 27 28 29 147 30 31 32 33 34 !40
& 35 36 33 37 38 39 40 41 42 43 !50
& 148 44 45 46 149 48 49 50 51 52 !60
& 53 54 55 47 56 57 150 58 59 60 !70
& 61 62 63 64 65 66 67 68 69 70 !80
& 60 71 72 73 74 75 77 78 79 80 !90
& 81 82 151 83 84 85 86 87 88 89 !100
& 90 91 92 93 94 95 96 97 98 99 !110
& 100 101 102 103 104 105 106 107 108 109 !120
& 110 111 112 113 114 115 116 117 152 118 !130
& 119 120 121 122 123 124 125 126 127 128 !140
& 7 9 136 137 9 138 139 76 140 141 !150
& 76 142 143 2 11 16 22 33 47 47 !160
& 78 108 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!node index number for node at outlet of segment
& 2 3 4 5 6 134 135 7 9 8 !10
& 9 11 12 13 5 14 9 16 17 18 !20
& 5 19 20 9 22 23 24 5 25 26 !30
& 27 28 29 2 30 31 9 33 34 35 !40
& 36 5 37 38 39 40 41 42 43 2 !50
```



```

& 44 45 9 47 48 49 50 51 52 53 !60
& 54 55 16 56 57 5 58 9 60 61 !70
& 62 63 64 65 66 67 68 69 70 23 !80
& 71 72 9 74 75 76 78 79 80 81 !90
& 82 5 83 84 9 86 87 9 89 90 !100
& 91 92 93 94 95 96 97 98 99 100 !110
& 101 102 47 104 105 106 76 108 109 110 !120
& 111 112 113 114 115 116 117 76 118 119 !130
& 120 121 122 123 124 125 126 127 128 76 !140
& 129 136 137 130 138 139 131 140 141 132 !150
& 142 143 133 144 145 146 147 148 149 150 !160
& 151 152 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!unique glaciation states
&! 1 Boral !Normal Boreal
&! 2 PrmT1 !Permafrost Talik
&! 3 IceC1 !Icesheet Coldbase
&! 4 PrmT0 !Permafrost No Talik
&! 5 IceW1 !Icesheet Warmbase
&! 6 ProL1 !Proglacial Lake
&! 7 Bora2 !Normal Boreal 2
&! 8 sta08 !state 8
&! 9 sta09 !state 9
&! 10 sta10 !state 10
&!identification of states with impermeable zone and pathway through
&! 0 = no impermeable zone
&! 1 = impermeable zone but no open pathway
&! 2 = impermeable zone with open pathway
& 0 0 0 0 0 0 0 0 0 0 !10
&!list of segments in open pathway passing through impermeable zone
& 0 0 0 0 0 0 0 0 0 0 !10
& 0 0 0 0 0 0 0 0 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
& 0 0 0 0 0 0 0 0 0 0 !60
& 0 0 0 0 0 0 0 0 0 0 !70
& 0 0 0 0 0 0 0 0 0 0 !80
& 0 0 0 0 0 0 0 0 0 0 !90
& 0 0 0 0 0 0 0 0 0 0 !100
& 0 0 0 0 0 0 0 0 0 0 !110
& 0 0 0 0 0 0 0 0 0 0 !120
& 0 0 0 0 0 0 0 0 0 0 !130
& 0 0 0 0 0 0 0 0 0 0 !140
& 0 0 0 0 0 0 0 0 0 0 !150
& 0 0 0 0 0 0 0 0 0 0 !160
& 0 0 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!lists of nodes
&!list of source nodes, last entry zero
& 1 10 15 21 32 46 59 77 85 88 !10
& 73 103 107 0 0 0 0 0 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
&!list of vault sector numbers connected to source nodes
& 1 2 3 4 5 6 7 8 9 10 !10
& 11 12 13 0 0 0 0 0 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
&!code number for vault release types
&!1 = AQUA (aqueous release)

```

```

&!2 = GAS (gaseous release)
& 1 1 1 1 1 1 1 1 1 1 !10
& 1 1 1 0 0 0 0 0 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
&!list of nodes in well aquifer
& 5 6 7 135 134 0 0 0 0 0 !10
& 0 0 0 0 0 0 0 0 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
& 0 0 0 0 0 0 0 0 0 0 !60
& 0 0 0 0 0 0 0 0 0 0 !70
& 0 0 0 0 0 0 0 0 0 0 !80
& 0 0 0 0 0 0 0 0 0 0 !90
& 0 0 0 0 0 0 0 0 0 0 !100
& 0 0 0 0 0 0 0 0 0 0 !110
& 0 0 0 0 0 0 0 0 0 0 !120
& 0 0 0 0 0 0 0 0 0 0 !130
& 0 0 0 0 0 0 0 0 0 0 !140
& 0 0 0 0 0 0 0 0 0 0 !150
& 0 0 0 0 0 0 0 0 0 0 !160
& 0 0 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!list of nonaquifer nodes for drawdown calculation
& 1 2 3 4 10 11 12 13 15 16 !10
& 17 18 21 22 23 24 25 26 27 28 !20
& 29 32 33 34 35 36 37 38 39 40 !30
& 41 42 43 46 47 56 57 149 48 49 !40
& 50 51 52 53 54 55 59 60 61 62 !50
& 63 64 65 66 67 68 69 70 77 78 !60
& 79 80 81 82 0 0 0 0 0 0 !70
& 0 0 0 0 0 0 0 0 0 0 !80
& 0 0 0 0 0 0 0 0 0 0 !90
& 0 0 0 0 0 0 0 0 0 0 !100
& 0 0 0 0 0 0 0 0 0 0 !110
& 0 0 0 0 0 0 0 0 0 0 !120
& 0 0 0 0 0 0 0 0 0 0 !130
& 0 0 0 0 0 0 0 0 0 0 !140
& 0 0 0 0 0 0 0 0 0 0 !150
& 0 0 0 0 0 0 0 0 0 0 !160
& 0 0 0 0 0 0 0 0 0 0 !170
& 0 0 0 0 0 0 0 0 0 0 !180
& 0 0 0 0 0 0 0 0 0 0 !190
& 0 0 0 0 0 0 0 0 0 0 !200
&!nodes in well aquifer bounding well position, upper then lower
& 153 5
&!list of biosphere discharge nodes
& 129 130 131 132 133 0 0 0 0 0 !10
&!code number for biosphere discharge
&!1 = AQUA (aquatic discharge)
&!2 = WELL (well discharge)
&!3 = TERR (terrestrial discharge)
&!4 = BOG (swamp or bog discharge)
&!5 = GAS (gaseous discharge)
&!9 = TOTL (a total discharge)
& 2 1 3 1 3 0 0 0 0 0 !10
&!list of nodes for determination of geosphere consequences
& 2 11 16 22 33 47 60 78 86 89 !10
& 74 104 108 129 130 131 132 133 0 0 !20
& 0 0 0 0 0 0 0 0 0 0 !30
& 0 0 0 0 0 0 0 0 0 0 !40
& 0 0 0 0 0 0 0 0 0 0 !50
& 0 0 0 0 0 0 0 0 0 0 !60

```

[illegible]

APPENDIX F: GEOSPHERE SORPTION INPUT DATA FILE

In this appendix is an extraction from the 4CS sorption input file. Only the data for 'Ac' is shown in order to show the general format of the file.

```
!
! SOR .FXD:
! 2011-Jul-28  VERSION 01A
! GEONET - SORPTION COEFFICIENT FIXED DATA FILE
! maximum number of nuclides = 40,  maximum number of elements = 25
! maximum number of minerals = 20,  maximum oxidation states = 2
! total of 10 coefficients for sorption/retardation equations
!
! coefficients entered in order
! b01      b02      b11      b22      b12
! b00      b03      b04      b05      b06
!
! for constant KD, coefficients b00, b03 and b06 are required
! b00 is the GM value for KD, default value zero giving unit retardation
! b03 is the size of variation from GM KD, default value zero for no variation
! b06 is the normalization factor to retardation factor, default value unity
!
!      Nuclide group HB
!
!  Ac (database subscript 1)
!  Am (database subscript 4)
!  Bi (database subscript 11)
!  C  (database subscript 14)
!  Ca (database subscript 15)
!  Cl (database subscript 19)
!  Cs (database subscript 23)
!  I  (database subscript 40)
!  Np (database subscript 58)
!  Pa (database subscript 62)
!  Pb (database subscript 63)
!  Po (database subscript 66)
!  Pu (database subscript 69)
!  Ra (database subscript 70)
!  Rn (database subscript 74)
!  Se (database subscript 79)
!  Tc (database subscript 86)
!  Th (database subscript 88)
!  U  (database subscript 92)
!
!
! 'AC' ! Data for element Ac
! SORC00(01,01,01)  oxidizing - granite ! g - Ac
&0.0      0.0      0.0      0.0      0.0
&3000      1.2      0.0      0.0      2.7
! SORC00(02,01,01)  reducing - granite ! g - Ac
&0.0      0.0      0.0      0.0      0.0
&3000      1.2      0.0      0.0      2.7
! SORC00(01,02,01)  oxidizing - montmorillon - Ac
&0.0      0.0      0.0      0.0      0.0
&150      1.3      0.0      0.0      2.6
! SORC00(02,02,01)  reducing - montmorillon - Ac
&0.0      0.0      0.0      0.0      0.0
&150      1.3      0.0      0.0      2.6
! SORC00(01,03,01)  oxidizing - gabbro ! ga - Ac
&0.0      0.0      0.0      0.0      0.0
```

```

&1500      1.2      0.0      0.0      2.7
!  SORC00(02,03,01)  reducing - gabbro ! ga - Ac
&0.0      0.0      0.0      0.0      0.0
&1500      1.2      0.0      0.0      2.7
!  SORC00(01,04,01)  oxidizing - overburden - Ac
&0.0      0.0      0.0      0.0      0.0
&2400      3        0.0      0.0      3.66
!  SORC00(02,04,01)  reducing - overburden - Ac
&0.0      0.0      0.0      0.0      0.0
&2400      3        0.0      0.0      3.66
!  SORC00(01,05,01)  oxidizing - sediment ! - Ac
&0.0      0.0      0.0      0.0      0.0
&5400      3        0.0      0.0      2.5
!  SORC00(02,05,01)  reducing - sediment ! - Ac
&0.0      0.0      0.0      0.0      0.0
&5400      3        0.0      0.0      2.5
!  SORC00(01,06,01)  oxidizing - biotite ! b - Ac
&0.0      0.0      0.0      0.0      0.0
&600      1        0.0      0.0      3.1
!  SORC00(02,06,01)  reducing - biotite ! b - Ac
&0.0      0.0      0.0      0.0      0.0
&600      1        0.0      0.0      3.1
!  SORC00(01,07,01)  oxidizing - calcite ! c - Ac
&0.0      0.0      0.0      0.0      0.0
&2000      0.5      0.0      0.0      2.7
!  SORC00(02,07,01)  reducing - calcite ! c - Ac
&0.0      0.0      0.0      0.0      0.0
&2000      0.5      0.0      0.0      2.7
!  SORC00(01,08,01)  oxidizing - chlorite ! - Ac
&0.0      0.0      0.0      0.0      0.0
...
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.
!  SORC00(00,00,00)  reducing - 18 - 25
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.
!  SORC00(00,00,00)  oxidizing - 19 - 25
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.
!  SORC00(00,00,00)  reducing - 19 - 25
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.
!  SORC00(00,00,00)  oxidizing - 20 - 25
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.
!  SORC00(00,00,00)  reducing - 20 - 25
&0.      0.      0.      0.      0.
&0.      1.      0.      0.      1.

```

APPENDIX G: SYVAC3-CC4 .PAR FILE

This appendix is an extraction from the 4CS median case .PAR file. This extraction shows only the general format of a .PAR file.

SV120801.PAR BEGUN 18-MAR-2011 16:28:43
Onfile - Based on Median Case 01 4CS

RUN NUMBER 1 (ACCEPT NUMBER) 1

SAMPLED AND CALCULATED PARAMETERS

1	AALPHA	ALPHA DOSE DISS. RATE EXPONENT	1.00000E+00	[]
2	ABETA	BETA DOSE DISS. RATE EXPONENT	1.00000E+00	[]
3	AGAMMA	GAMMA DOSE DISS. RATE EXPONENT	1.00000E+00	[]
4	ALFCOF	ALPHA FUEL DOSE VARY FACTOR	1.00000E+00	[]
5	ALPHDO (01)	FUEL ALPHA DOSE RATES DAT01	1.42000E+06	[GY/A]
6	ALPHDO (02)	FUEL ALPHA DOSE RATES DAT02	1.72000E+06	[GY/A]
7	ALPHDO (03)	FUEL ALPHA DOSE RATES DAT03	1.89000E+06	[GY/A]
8	ALPHDO (04)	FUEL ALPHA DOSE RATES DAT04	1.99000E+06	[GY/A]
9	ALPHDO (05)	FUEL ALPHA DOSE RATES DAT05	2.03000E+06	[GY/A]
10	ALPHDO (06)	FUEL ALPHA DOSE RATES DAT06	2.05000E+06	[GY/A]
11	ALPHDO (07)	FUEL ALPHA DOSE RATES DAT07	2.04000E+06	[GY/A]
12	ALPHDO (08)	FUEL ALPHA DOSE RATES DAT08	2.00000E+06	[GY/A]
13	ALPHDO (09)	FUEL ALPHA DOSE RATES DAT09	1.88000E+06	[GY/A]
14	ALPHDO (10)	FUEL ALPHA DOSE RATES DAT10	1.77000E+06	[GY/A]
15	ALPHDO (11)	FUEL ALPHA DOSE RATES DAT11	1.58000E+06	[GY/A]
16	ALPHDO (12)	FUEL ALPHA DOSE RATES DAT12	1.30000E+06	[GY/A]
17	ALPHDO (13)	FUEL ALPHA DOSE RATES DAT13	9.03000E+05	[GY/A]
18	ALPHDO (14)	FUEL ALPHA DOSE RATES DAT14	3.21000E+05	[GY/A]
19	ALPHDO (15)	FUEL ALPHA DOSE RATES DAT15	1.80000E+04	[GY/A]
20	ALPHDO (16)	FUEL ALPHA DOSE RATES DAT16	6.24000E+03	[GY/A]
21	ALPHDO (17)	FUEL ALPHA DOSE RATES DAT17	4.19000E+03	[GY/A]
...				
34290	WCNLIM (031,18)	WARN: CONC GT CNLIM Th230 caoup	0.00000E+00	[]
34291	WCNLIM (032,18)	WARN: CONC GT CNLIM Th231 caoup	0.00000E+00	[]
34292	WCNLIM (033,18)	WARN: CONC GT CNLIM Th232 caoup	0.00000E+00	[]
34293	WCNLIM (034,18)	WARN: CONC GT CNLIM Th234 caoup	0.00000E+00	[]
34294	WCNLIM (035,18)	WARN: CONC GT CNLIM U 233 caoup	0.00000E+00	[]
34295	WCNLIM (036,18)	WARN: CONC GT CNLIM U 234 caoup	0.00000E+00	[]
34296	WCNLIM (037,18)	WARN: CONC GT CNLIM U 235 caoup	0.00000E+00	[]
34297	WCNLIM (038,18)	WARN: CONC GT CNLIM U 236 caoup	0.00000E+00	[]
34298	WCNLIM (039,18)	WARN: CONC GT CNLIM U 238 caoup	0.00000E+00	[]
34299	WCNLIM (040,18)	WARN: CONC GT CNLIM dumn1 caoup	0.00000E+00	[]

APPENDIX H: SYVAC3-CC4 .DOS FILE

This appendix contains an entire .DOS file for a 4CS reference case.

```
SV120801.DOS          BEGUN  18-MAR-2011  16:28:43
Onfile - Based on Median Case 01 4CS
Calculation order for Geosphere network nodes:
  89  90  91  92  93      94  95  96  97  98
  99 100 101 102 60      47  61 149 108 62
  48  33 152  63  49      37 118  64  50  38
  22 119  65  51  39      25 120 109  66  52
  40  26 121 110  67      53  41  27 122 111
  78  68  54  42  28      123 112  79  69  55
  43  29 124 113  80      34  70  16  11  2
 125 114  81  56  35      23  17  12  3 126
 115 104 151 148 147      146  82  57  36  24
  18  13  4 127 116      105  74  86  83  71
 150  44  30  19 145      144  5 128 117 106
  75  87  84  72  58      45  31  20  14  8
   6  76  9 134 142      140 138 136 135 143
 141 139 137  7 133      132 131 130 129  0
   0  0  0  0  0        0  0  0  0  0
   0  0  0  0  0        0  0  0  0  0
   0  0  0  0  0        0  0  0  0  0
   0  0  0  0  0        0  0  0  0  0
   0  0  0  0  0        0  0  0  0  0
   0  0  0  0  0        0  0  0  0  0
  RUN #      1 ***** RUN #      1 ***** RUN #      1
***** RUN #      1 *****
MAXIMUM DOSE FROM ALL NUCLIDES UP TO TLIMIT (MXLDA):  9.71311D-08 Sv/a at (TMXLDA):
1.10450D+06 a
MAXIMUM DOSE FROM ALL NUCLIDES UP TO 1.00000D+06a (MXTDA):  9.62262D-08 Sv/a at
(TMXTDA):  1.00000D+06 a
TOTAL DOSE (DDT [Sv/a]) FROM EACH NUCLIDE AT TMXTDA ( 1.00000D+06 a)
  PU240AFUEL  0.0000D+00  AC225AFUEL  0.0000D+00  TH231AFUEL  0.0000D+00
  U 236AFUEL  0.0000D+00  PU242AFUEL  0.0000D+00  PA231AFUEL  0.0000D+00
  TH232AFUEL  0.0000D+00  U 238AFUEL  0.0000D+00  AC227AFUEL  0.0000D+00
  RA228AFUEL  0.0000D+00  TH234AFUEL  0.0000D+00  TH227AFUEL  0.0000D+00
  TH228AFUEL  0.0000D+00  U 234AFUEL  0.0000D+00  RA223AFUEL  0.0000D+00
  RA224AFUEL  0.0000D+00  TH230AFUEL  0.0000D+00  BI208 FUEL  2.1365D-15
  PU241AFUEL  0.0000D+00  RA226AFUEL  0.0000D+00  C 14 FUEL  0.0000D+00
  AM241AFUEL  0.0000D+00  RN222AFUEL  0.0000D+00  CA 41 FUEL  2.5430D-14
  NP237AFUEL  0.0000D+00  PB210AFUEL  0.0000D+00  CL 36 FUEL  7.7803D-11
  PA233AFUEL  0.0000D+00  BI210AFUEL  0.0000D+00  CS135 FUEL  0.0000D+00
  U 233AFUEL  0.0000D+00  PO210AFUEL  0.0000D+00  I 129 FUEL  9.6148D-08
  TH229AFUEL  0.0000D+00  PU239AFUEL  0.0000D+00  SE 79 FUEL  2.0471D-14
  RA225AFUEL  0.0000D+00  U 235AFUEL  0.0000D+00  TC 99 FUEL  0.0000D+00
PEAK DOSE (MXLDT [Sv/a]) FROM EACH NUCLIDE AT TMXLDT ([a])
  PU240AFUEL  0.0000D+00 at 1.0000D+07  AC225AFUEL  0.0000D+00 at 1.0000D+07
  TH231AFUEL  0.0000D+00 at 1.0000D+07
  U 236AFUEL  0.0000D+00 at 1.0000D+07  PU242AFUEL  0.0000D+00 at 1.0000D+07
  PA231AFUEL  0.0000D+00 at 1.0000D+07
  TH232AFUEL  0.0000D+00 at 1.0000D+07  U 238AFUEL  0.0000D+00 at 1.0000D+07
  AC227AFUEL  0.0000D+00 at 1.0000D+07
  RA228AFUEL  0.0000D+00 at 1.0000D+07  TH234AFUEL  0.0000D+00 at 1.0000D+07
  TH227AFUEL  0.0000D+00 at 1.0000D+07
  TH228AFUEL  0.0000D+00 at 1.0000D+07  U 234AFUEL  0.0000D+00 at 1.0000D+07
  RA223AFUEL  0.0000D+00 at 1.0000D+07
  RA224AFUEL  0.0000D+00 at 1.0000D+07  TH230AFUEL  0.0000D+00 at 1.0000D+07
  BI208 FUEL  4.2392D-15 at 1.6171D+06
  PU241AFUEL  0.0000D+00 at 1.0000D+07  RA226AFUEL  0.0000D+00 at 1.0000D+07
  C 14 FUEL  5.6226D-16 at 9.2778D+04
```

AM241AFUEL	0.0000D+00	at	1.0000D+07	RN222AFUEL	0.0000D+00	at	1.0000D+07
CA 41 FUEL	3.4347D-14	at	8.0000D+05	PB210AFUEL	0.0000D+00	at	1.0000D+07
NP237AFUEL	0.0000D+00	at	1.0000D+07	BI210AFUEL	0.0000D+00	at	1.0000D+07
CL 36 FUEL	1.3942D-10	at	5.6836D+05	PO210AFUEL	0.0000D+00	at	1.0000D+07
PA233AFUEL	0.0000D+00	at	1.0000D+07	PU239AFUEL	0.0000D+00	at	1.0000D+07
CS135 FUEL	4.0934D-14	at	1.0000D+07	U 235AFUEL	0.0000D+00	at	1.0000D+07
U 233AFUEL	0.0000D+00	at	1.0000D+07				
I 129 FUEL	9.7069D-08	at	1.1045D+06				
TH229AFUEL	0.0000D+00	at	1.0000D+07				
SE 79 FUEL	9.8177D-14	at	3.8555D+06				
RA225AFUEL	0.0000D+00	at	1.0000D+07				
TC 99 FUEL	0.0000D+00	at	1.0000D+07				

MAXIMUM ELEMENT CONCENTRATIONS

ELEMENT	WELL WATER [mol/m3]	TIME [a]	LAKE WATER [mol/m3]	TIME [a]
AC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
AM	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
BI	1.4980D-18	1.6177D+06	2.3656D-23	1.6109D+06
C	1.6112D-20	9.2778D+04	2.5436D-25	9.2812D+04
CA	3.8393D-16	8.0000D+05	6.0687D-21	8.0000D+05
CL	1.7175D-12	5.6836D+05	2.7143D-17	5.6750D+05
CS	9.2986D-16	1.0000D+07	1.4688D-20	1.0000D+07
I	6.8914D-10	1.1045D+06	1.0877D-14	1.1045D+06
NP	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PB	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PO	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RN	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
SE	2.2727D-16	3.8803D+06	3.5875D-21	3.8555D+06
TC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
TH	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
U	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
DU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07

ELEMENT	SOIL [mol/kg]	TIME [a]	LAKE SEDIMENT [mol/kg]	TIME [a]
AC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
AM	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
BI	1.0669D-19	1.6171D+06	0.0000D+00	1.0000D+07
C	7.7893D-25	9.2500D+04	0.0000D+00	1.0000D+07
CA	1.3868D-18	8.0000D+05	0.0000D+00	1.0000D+07
CL	2.0414D-16	5.6750D+05	0.0000D+00	1.0000D+07
CS	1.7904D-16	1.0000D+07	0.0000D+00	1.0000D+07
I	3.3549D-12	1.1045D+06	0.0000D+00	1.0000D+07
NP	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PB	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PO	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RN	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
SE	4.0038D-18	3.8555D+06	0.0000D+00	1.0000D+07
TC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
TH	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
U	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
DU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07

ELEMENT	INDOOR AIR [mol/m3]	TIME [a]	OUTDOOR AIR [mol/m3]	TIME [a]
AC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
AM	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
BI	4.3914D-24	1.6177D+06	6.2967D-27	1.6190D+06
C	5.6706D-24	9.2778D+04	1.9140D-27	9.2500D+04
CA	1.1239D-21	8.0000D+05	8.1821D-26	8.0000D+05
CL	5.0275D-18	5.6836D+05	4.6978D-23	5.6750D+05
CS	2.7325D-21	1.0000D+07	1.0563D-23	1.0000D+07
I	2.0303D-15	1.1045D+06	1.2987D-17	1.1045D+06
NP	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PB	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07

PO	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
PU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RA	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
RN	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
SE	6.6552D-22	3.8803D+06	2.3623D-25	3.8555D+06
TC	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
TH	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
U	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07
DU	0.0000D+00	1.0000D+07	0.0000D+00	1.0000D+07

APPENDIX I: SYVAC3-CC4 .LPT FILE

This appendix is an extraction from a median case .LPT file. This extraction shows only the general format of the .LPT file.

```
SV120801.LPT          BEGUN  29-JUL-2011  13:29:31

* * * * *
*
*                               CC4
*
*       CC4 Model Code - version 4.08
*       Version CC4.08 changes Copyright(C) 2010
*       Version CC4.07 changes Copyright(C) 2008
*       by Nuclear Waste Management Organization
*
*       Version CC4.06 changes Copyright(C) 2006
*       Version CC4.05 changes Copyright(C) 2005
*       Version CC4.04 changes Copyright(C) 2003
*       Version CC4.03 changes Copyright(C) 2002
*       by Ontario Power Generation Limited
*
*       Version CC4.02 Copyright(C) 2001 by
*       Atomic Energy of Canada Ltd.(AECL)
*
* * * * *
*
*                               SYVAC3
*
*       Systems Variability Analysis Code - version 3.12
*
*       Version SV3.12 changes Copyright(C) 2010
*       by Nuclear Waste Management Organization
*
*       Version SV3.11 changes Copyright(C) 2005
*       by Ontario Power Generation Limited
*
*       Version SV3.10 Copyright(C) 1987,1988,1989,1990,
*                               1991,1995,1996
*       by Atomic Energy of Canada Ltd. (AECL)
*
*       AECL Proprietary Information
*
*       All Rights Reserved
*
* * * * *

TITLE:
Median - HB00 2011 - 07 - 29

LOWEST RUN NUMBER ===== 1
HIGHEST RUN NUMBER ===== 1
NUMBER OF RUN NUMBER RANGES ===== 1
NUMBER OF ACCEPTED RUNS REQUESTED ==== 1
```

```

OUTPUT TYPE ===== SHORT
OPTIONAL FILES ===== PAR SUB NDS CDS
MINIMUM NUMBER OF TIME STEPS ===== 3
MAXIMUM NUMBER OF TIME STEPS ===== 200
TARGET FRACTIONAL ERROR ===== 1.000000D-03
SMOOTHING COEFFICIENT (TIMES ) ===== 2.000000D-01
SMOOTHING COEFFICIENT (VALUES) ===== 2.000000D-01
NUMBER OF FIXED TIMES ===== 26

FIXED TIMES:
      0.00000      10.0000      18.0000      32.0000      56.0000
      100.000      180.000      320.000      560.000      1000.00
      1800.00      3200.00      5600.00      10000.0      18000.0
      32000.0      56000.0      100000.      180000.      320000.
      560000.      1.000000E+06  1.800000E+06  3.200000E+06  5.600000E+06
      1.000000E+07

COMMON BLOCKS OF PARAMETERS IN INCLUDE FILES ARE:
CQCNTA.INC
/CQCNTA/
...
SPWTDG.INC
/SPWTDG/

SAMPLING METHOD ===== QUANTILE
SAMPLING FILE NAME ===== MEDIANHB.QNT

PARAMETERS SAMPLED BY QUANTILE ARE:
ALPHA DOSE DISS. RATE EXPONENT      AALPHA      []
CONST      value =      1.000000D+00
...
INSTANT RELEASE FRAC. DUMN1      IRFRV(040)      []
CONST      value =      0.000000D+00

SAMPLING METHOD ===== CALCULATED
CALCULATED PARAMETERS ARE:
SECTOR BUFFER DARCY VEL.      sec01      DARBV(01)      [M/A]      S      1
...
SEDIM" T DIST. COEFF      dis10 dume6      SEDKD(10,25)      [L/KG]      N      1

SAMPLING METHOD ===== CONSEQUENCES
CONSEQUENCES ARE:
AMT ACCUM. IN FAILED CONT. Ac225      AMTCNT(001)      [MOL]      S      1
NUM      -1.0
...
WARN: CONC > CNLIM      dumn1 caout      WCNLIM(040,12)      []      N      1
INT      -1

CHAINS: (ONE PER LINE. "=" INDICATES SECULAR EQUILIBRIUM WITH PREVIOUS NUCLIDE.)

PU240AFUEL U 236AFUEL TH232AFUEL =RA228AFUEL =TH228AFUEL =RA224AFUEL
PU241AFUEL AM241AFUEL NP237AFUEL =PA233AFUEL U 233AFUEL TH229AFUEL
=RA225AFUEL =AC225AFUEL
PU242AFUEL U 238AFUEL =TH234AFUEL U 234AFUEL TH230AFUEL RA226AFUEL
=RN222AFUEL =PB210AFUEL =BI210AFUEL =PO210AFUEL
PU239AFUEL U 235AFUEL =TH231AFUEL PA231AFUEL =AC227AFUEL =TH227AFUEL
=RA223AFUEL
BI208 FUEL
C 14 FUEL

```

CA 41 FUEL
CL 36 FUEL
CS135 FUEL
TC 99 FUEL
SE 79 FUEL
I 129 FUEL
MATRIX MATERIALS:
U 238AFUEL

4245 SAMPLED PARAMETERS ARE CONSTANT
6894 SAMPLED AND CALCULATED PARAMETERS VARY
20195 CONSEQUENCES

RECORD LENGTH = 132 BYTES.
--WARNING IN RUN # 1 -- (SIMLAT)
BEGINNING SIMULATION

SUMMARY OF RANGE NUMBER =====	1
STARTING RUN NUMBER =====	1
ENDING RUN NUMBER =====	1
NUMBER OF ACCEPTED RUNS REQUESTED =====	1
NUMBER OF RUNS ACCEPTED =====	1
NUMBER OF RUNS ON HOLD =====	0
NUMBER OF RUNS REJECTED =====	0

NUCLIDE ACCEPTANCE:

NUCLIDE	# RUNS	% OF ACCEPTED RUNS
PU240AFUEL	1	100.00
U 236AFUEL	1	100.00
TH232AFUEL	1	100.00
RA228AFUEL	1	100.00
TH228AFUEL	1	100.00
RA224AFUEL	1	100.00
PU241AFUEL	1	100.00
AM241AFUEL	1	100.00
NP237AFUEL	1	100.00
PA233AFUEL	1	100.00
U 233AFUEL	1	100.00
TH229AFUEL	1	100.00
RA225AFUEL	1	100.00
AC225AFUEL	1	100.00
PU242AFUEL	1	100.00
U 238AFUEL	1	100.00
TH234AFUEL	1	100.00
U 234AFUEL	1	100.00
TH230AFUEL	1	100.00
RA226AFUEL	1	100.00
RN222AFUEL	1	100.00
PB210AFUEL	1	100.00
BI210AFUEL	1	100.00
PO210AFUEL	1	100.00
PU239AFUEL	1	100.00
U 235AFUEL	1	100.00
TH231AFUEL	1	100.00
PA231AFUEL	1	100.00
AC227AFUEL	1	100.00
TH227AFUEL	1	100.00
RA223AFUEL	1	100.00
BI208 FUEL	1	100.00
C 14 FUEL	1	100.00
CA 41 FUEL	1	100.00
CL 36 FUEL	1	100.00
CS135 FUEL	1	100.00
TC 99 FUEL	1	100.00
SE 79 FUEL	1	100.00

I 129 FUEL 1 100.00

CASE FINISHED AT RUN NUMBER: 1, WITH:
 1 ACCEPTED RUNS,
 0 REJECTED RUNS, AND
 0 RUNS ON HOLD.

CASE ENDED AT 13-MAR-2009 09:21:03
CPU TIME 0 HR 27.74 MIN

DOING:	%	CPU TIME (DURING PRESENT EXECUTION)
INPUT	2.40%	39.94
SELECTION	0.17%	2.86
SOURCE	0.00%	0.00
RESPONSE	0.00%	0.00
CONVOLUTION	0.00%	0.00
RESULT	97.43%	1621.62
CONSEQUENCE	0.00%	0.00

APPENDIX J: PROGRAMMER GUIDE

J.1 INTRODUCTION TO PROGRAMMER GUIDE

Since the CC4 code runs under the SYVAC3 executive, it is structured to follow SYVAC3 conventions. This Appendix provides information relevant to programmers or advanced users on specific topics. The user is referred to the SYVAC3 Manual (Andres, 2000) for further details.

J.2 INCLUDE FILES

Model variables that are shared with SYVAC3 must be one of the four SYVAC3 classes: sampled, dependent, consequence or time series.

Sampled parameters, dependent parameters and consequence parameters are declared and assigned to common blocks in INCLUDE files with names beginning with "SP", "DP" and "CQ" respectively. These INCLUDE files must be available to SYVAC3 during execution of the code, because SYVAC3 needs to know where the variables are stored. A specific format for such files has been developed:

- The common block names must start with "SP" for sampled parameters, "DP" for dependent parameters and "CQ" for consequences (time series are not declared in these common blocks). Names cannot exceed six characters in length.
- Each common block can be accessed by a vector with the same name as the common block. The length of this vector is provided by a parameter with a name that is similar to that of the common block name. The name of the length parameter is formed by deleting the 2nd character of the common block name and prefixing the remaining characters with an "L" (e.g., DPTRAN to LDTRAN). The vector provides access to the common block by means of the Fortran EQUIVALENCE instruction. That is, every variable in the common block can be accessed in two ways - by its variable name, and by the equivalent vector.
- Variables in the common block must have their dimensions (if any) declared in the COMMON statement, not in a type declaration or DIMENSION statement.
- All variables in a common block must have the same type, either INTEGER or DOUBLE PRECISION.
- Contents of each common block must be preserved by a SAVE statement (essential on some computers, but not others).

It is recommended that array variable dimensions be given fixed values in Fortran PARAMETER statements. This allows all array sizes to be changed simply by changing one PARAMETER statement.

J.3 NUCLIDE AND CHAIN LISTS

Sampled parameters, dependent parameters and consequence parameters may be nuclide-dependent. The number of such nuclides is defined by the parameter MXSPEC. The nuclide index from this parameter list is called NUCPAR by convention.

However, while the input parameters (and dependent and consequence parameters) will be indexed according to a given set of nuclides, SYVAC3 allows the user to specify a subset of these nuclides to simulate in a given run. Since this subset also contains the decay chain relationships between these nuclides, these nuclides are referred to as the "chains list". The same nuclide will in general have a different index in the main input parameter list than in the chains list. By convention, the chains list index is called NUCCHN. NUCCHN varies between 1 and NNUC, where NNUC is between 1 and MXSPEC.

SYVAC3 restricts the radionuclide decay chains modelled to linear sequence of nuclides. A nuclide in a decay chain can be linked to at most two other nuclides, its parent and its daughter. All the nuclides up to and including a given nuclide in a decay chain are known collectively as its precursors (or parents). All the nuclides that following a nuclide in a decay chain, including the nuclide itself, are known as its descendents (or daughters).

Table J.1 shows some arrays SYVAC3 provides in NUCLID.INC. The array sizes are given in terms of Fortran parameters provided by SYVAC3, which are listed in Table J.2.

SYVAC3 has representations for chemical elements and matrix materials (i.e., wasteforms) as well as nuclides and chains. The element type represents chemical element, such as carbon or uranium. The matrix material type represents the wasteform in which nuclides are embedded.

Table J.3 shows the SYVAC3 arrays that implement the associations between nuclide, element, and matrix material types. The dimensioning constants are defined in Table J.2.

J.4 TIME SERIES

Time series are sets of (time, value) points that define a time-dependent variable. The times and values are double precision floating point. Time series are accessed by the system model through integer indexes that identify a specific time series (maintained automatically by SYVAC3). Time series names can contain no more than six characters. The SYVAC3 Time Series Package provides a number of routines for time-series operation - for example, addition of two time series.

During the construction of a new Time Series, the Time Series Package may call a user routine many times. Since the user routine is called directly by the Time Series Package, it must have a standard interface that is defined in the SYVAC3 Manual (Andres, 2000). The SV311 source code directories also contains templates for user routines in the IFCODE (InterFace) area.

A user routine defines some system submodel function of time. It must be able to provide both appropriate time point estimates as well as accurate values of the function at any given time point. The time point estimates should be close to the local extrema of the time function in order to ensure that the Time Series Package does not overlook any important features of the function.

SYVAC3 stores Time Series as a large collection of Time Series objects. A system model accesses stored Time Series via a numerical index called a handle. Even with a large array dimension, some large models run out of storage space. Since the Time Series Package has no way of knowing which old Time Series are no longer needed, it simply deletes the oldest time series first in order to make room for new ones.

J.5 ASSIGNING VALUES TO DEPENDENT PARAMETERS (DEPPAR)

After reading the input file and setting up the general variable arrays and common blocks, SYVAC3 calls a system model FORTRAN routine called DEPPAR.FOR. The primary function of DEPPAR is to calculate the values of dependent parameters before any time-dependent calculations are performed.

DEPPAR also sets certain parameters which indicate how a nuclide is to be treated in a given simulation. Specifically, it sets NUCSIM(NUCCHN) to 'FALSE' if it is determined that the nuclide indexed by NUCCHN should not be simulated – e.g., if the inventory is negligibly small. It also increments NUCUSE(NUCCHN) once each simulation to indicate how many times NUCCHN was simulated in a given run.

Another function of DEPPAR is to check the input and dependent parameters to ensure that they fall within the domain of application of the model.

J.6 RUN SYSTEM MODEL (SIMLAT)

The top-level system model routine SIMLAT.FOR is called by SYVAC3 to run the time-dependent system model for one simulation, with a defined set of sampled values provided for all input parameters, calculated values for dependent parameters, default values for consequence parameters, and time series reset. SIMLAT then calls further FORTRAN modules to perform the model calculations.

In the course of the calculations, control may be passed back and forth between lower-level SYVAC3 and system model routines, but eventually control is passed back to SIMLAT. When the simulation is finished, SIMLAT returns control to SYVAC3, which then writes results to output files and, if requested, sets up for another simulation starting with re-sampling the input parameters. It is recommended practice to call the SYVAC3 routine ZAPTSS to initialize the time series between simulations, otherwise it is possible that time series might become contaminated by time series from previous simulations. ZAPTSS also resets the time series storage space so it need hold only the time series generated in one simulation.

Simulations may run into problems for various reasons. Simulations may be rejected, put on-hold or accepted. The values of logical arguments returned by DEPPAR and SIMLAT determine these states. Table J.4 summarizes the meanings and consequences of the combinations of states of the ACCEPT (DEPPAR) and ONHOLD (SIMLAT) flags.

The SYVAC3 routine STRACE is used to turn on and off the tracing of time series operations. Tracing time series operations is a good way of understanding how they work, but the files generated can get very large.

Table J.1: SYVAC3 Nuclide and Chain Variables

Array Name	Type	Dimensions	Description, $1 \leq n = \text{NUCCHN} \leq \text{NNUC}$
FSENUC	INTEGER	MXSPEC	If SECEQU(n) is .TRUE., then FSENUC(n) is a number in the set [1, n] identifying the first nuclide in a secular equilibrium relationship with n; otherwise FSENUC(n) = 0.
NNUC	INTEGER	scalar	Total number of nuclides in all chains read from the input file for the current case; $1 \leq \text{NNUC} \leq \text{MXSPEC}$.
NOPRE	INTEGER	MXSPEC	NOPRE(n) is the number of precursors of nuclide n, including n itself; $\text{NOPRE}(n) \geq 1$.
NUCID	CHAR*10	MXSPEC	NUCID(n) is the name of nuclide n, including a wasteform identifier.
NUCSIM	LOGICAL	MXSPEC	NUCSIM(n) is .TRUE. if nuclide n is to be simulated in the current simulation and .FALSE. Otherwise; it must be set by the model.
NUCUSE	INTEGER	MXSPEC	NUCUSE(n) is a count of the simulations in the current case so far in which nuclide n was simulated fully; it must be updated by the model.
PREIDX	INTEGER	MAXLCH, MXSPEC	PREIDX(i,n) is the i'th precursor of nuclide n, for i from 1 to NOPRE(n); $1 \leq \text{PREIDX}(i,n) \leq \text{NOPRE}(n)-i+1$, and $\text{PREIDX}(\text{NOPRE}(n),n) = n$.
SECEQU	LOGICAL	MXSPEC	SECEQU(n) is .TRUE. only if nuclide n is in secular equilibrium with another nuclide.

Table J.2: SYVAC3 (Version SV312) Nuclide, Element and Matrix Dimensioning Parameters

Constant	Include File (.INC)	SYVAC3 Package	Description	Value
MAXLCH	MAXLCH	TS	Maximum length of any nuclide decay chain	10
MXSPEC	MXSPEC	SV	Maximum number of nuclide species allowed in a case	40
MXCHEM	MXCHEM	EC	Maximum number of chemical elements among nuclides allowed in a case	25
MXMTRX	MXMTRX	SV	Maximum number of matrix materials	2

Table J.3: SYVAC3 Element and Matrix Material Arrays

Include File	Array Name	Type	Dimension	Description, where n is a valid nuclide (chain) index, e is a valid element index and m is a valid matrix material index
ELMID	ELMID	CHAR*2	MXCHEM e.g., I, Kr, U, Th	ELMID(e) is the name of the e'th element.
MATRIX	MATRX	CHAR*4	MXMTRX	MATRX(m) is the name of the m'th matrix material; e.g., FUEL, ZRLY.
	MIDXN	INTEGER	MXMTRX	MIDXN(m) is a nuclide number, pointing to a nuclide with properties that define those of the m'th wasteform
	MIDXP	INTEGER	MXSPEC	MIDXP(m) is a nuclide number, pointing to the nuclide in parameter order with properties that define those of the m'th wasteform
	NMATRX	INTEGER	scalar	Number of matrix materials in the input chains list; 1 <= NMATRX <= MXMTRX.
NUCIDX	ELMIDX	INTEGER	MXSPEC	ELMIDX(n) is an element index between 1 and NELMNT indicating the element to which nuclide n belongs.
	NIDXM	INTEGER	MXSPEC	NIDXM(n) is a matrix material index between 1 and NMATRX indicating where nuclide n is found.
	NELMNT	INTEGER	scalar	Number of elements among the nuclides in the input file.

Table J.4: SYVAC3 Simulation Status Flags

ACCEPT (DEPPAR)	ONHOLD (SIMLAT)	Simulation State	Sampled Parameters Status	Dependent Parameters Status	Consequence Parameters Status
.FALSE.	(NA)	Rejected	Sampled normally	Not defined	Artificial values
.TRUE.	.TRUE.	On hold	Sampled normally	Calculated normally	Very large values
.TRUE.	.FALSE.	Accepted	Sampled normally	Calculated normally	Calculated normally

APPENDIX K: INSTALLATION OF SYVAC3-CC4

K.1 SOURCE CODE

The SYVAC3-CC4 reference source code (FORTRAN and INCLUDE files) should be obtained from an official source and placed under configuration management in the user's software system.

The current version of SYVAC3-CC4 is made up of the following software packages:

- SV312 (SYVAC generation 3, version 12),
- CC408 (Disposal system model, generation 4, version 8),
- ML303 (Modeling Library generation 3, version 3), and
- SLATEC (SLATEC numerical algorithm library, version 4.1, July 1993).

The reference version of the SYVAC3 source code, SV312, contains the following code packages:

- ECcode - SYVAC Executive Control code,
- FRcode - SYVAC File Reading code,
- PScode - SYVAC Parameter Sampling code,
- SVcode - SYVAC General Fortran code,
- TScode - SYVAC Time Series Fortran code, and
- IFcode - interface routines for coupling a new system model to SYVAC (not needed for compiling the existing system model).

The reference version of the disposal system model, CC408, contains the following code packages:

- VTcode - INROC vault model,
- BTcode - BIOTRAC biosphere transport model,
- DOcode - BIOTRAC dose calculation model,
- F3code – FRAC3DVS interface for CC4,
- GTcode - GEONET geosphere transport model, and
- CCcode - Common code between the above packages and for interfaces with SYVAC3.

The reference version of the Modelling Library source code, ML303, contains the following code packages:

- ARcode - Assorted Routines code,
- FIcode - Finite Interval response function code, and
- SIcode - Semi-Infinite response function code.

The reference version of the SLATEC source code is one package called SLATEC, which is normally kept with the CC403 code package.

K.2 CREATION OF EXECUTABLE FOR WINDOWS

There are many ways to create a correct version of the SYVAC3-CC4 executable file. This manual will only discuss two methods, referred to as "Code Accumulation" and "Search List" respectively. The following description applies to creating an executable using the Compaq Visual FORTRAN Professional Edition Version 6.6 and Version 11.1 running under Windows.

Whichever method is used, the resulting executable should be installed under configuration management in the user's software system, and verified against appropriate reference runs.

Code Accumulation

The first task in creating an executable when using "Code Accumulation" is to collect all required source code into one directory. This must be done in the correct order so that the correct version of each code is used. In particular, some SYVAC3 INCLUDE files are overwritten by CC4 versions that, for example, change default SYVAC3 array dimensions to values appropriate for CC4. The recommended order for copying in all *.FOR and *.INC files is as follows:

- SV312 (copy in order ECcode, FRcode, PScode, SVcode, and TScode),
- ML303 (copy in order ARcode, FIcode, SIcode), and
- CC408 (copy in order SLATEC, BTcode, DOcode, GTcode, F3code, VTcode, and CCcode).

Next the code must be compiled and linked. The Compaq or Intel Visual FORTRAN User Guide has complete documentation on compiling and linking a simple project with all files in one directory. No changes are required to the compiler settings with FORTRAN v6.6 for either the release or debug version of the executable. The Intel version 11.1 compiler needs the following flags either selected through the GUI interface under the project settings under the FORTRAN tab or as additional commands in the command line tab:

- /Qsave, saves all values in a subroutine call for the next time the subroutine is called,
- /stand:f90, to enforce Fortran 90 standards, and
- check routine interfaces is set to NO, (can set it to yes for checking and debugging).

The detailed comparison of the compiler settings for Compaq Visual Fortran 6.6 and Intel Visual Fortran 11.1 are provided in Table K.1. Under Project settings in both cases, the FORTRAN tab was selected and all the sub items compared. The common items are highlighted in yellow within each category. The items not quite the same are highlighted in blue. Green items change in experiments.

Table K.1: Fortran Compiler Comparison

Compaq Visual Fortran 6.6	Intel Visual Fortran 11.1
GENERAL	GENERAL
Debugging level: full	Suppress Banner: Yes (/nologo)
Warning level: normal warnings*	Additional include directories: blank
Optimization level: none	Debug information format: full(/debug:full)
Pre-defined preprocessor symbols:blank	Optimization: Disable(/Od)
Generate Source browse information: not checked	Preprocessor Definitions: blank
	Compile Time diagnostics: Custom

Compaq Visual Fortran 6.6	Intel Visual Fortran 11.1
Common Options: inheritance description not available	
CODE GENERATION	CODE GENERATION
Generate most-optimized code: blank Enable recursive routines: blank Math library: Check* Generate code for: Blend* Common Options: inheritance description not available	Enable recursive routines: No Generate Reentrant code: default Object String: blank Enable Enhanced Instruction Set: not set Add Processor-Optimized code path: none Intel Processor-Specific optimization: none
COMPATIBILITY	COMPATIBILITY
Unformatted file conversion: None* Enable VMS compatibility: blank Enable F77 run-time compatibility: blank Enable F77 integer constants: blank Powerstation 4.0 compatibility options: just Libraries checked Common Options: inheritance description not available	Unformatted file conversion: None Enable VMS compatibility: no Enable F77 run-time compatibility: no Enable F77 integer constants: no Powerstation 4.0 compatibility options: just Libraries "yes" rest no
COMPILATION DIAGNOSTICS	DIAGNOSTICS (diff title)
Error limit: blank Warning level: Normal Warnings* Things checked: Argument mismatch Data alignment Uncalled routines Uninitialized variables Usage Fortran Standards checking : None* Common Options: inheritance description not available	GENERAL Error limit: 30 Treat Warnings as errors: No Warn for non-standard Fortran: No Treat Fortran Standard warnings as Errors: No OpenMP Diagnostic level: default Auto-Parallelizer Diagnostic Level: Default Vectorizer Diagnostic level: Default Disable specific diagnostics: blank Emit diagnostics to file: No Diagnostics file: \$(IntDir)\\$(TargetName).diag Generate Interface Blocks: Yes(/gen-interfaces) LANGUAGE USAGE Compile time Diagnostics: Custom Warn for Undeclared symbols : No Warn for Unused Variables: No Warn When removing %LOC: No Warn When truncating source line: No Warn for Unaligned data: Yes Warn for Uncalled Statement Function: No Suppress Usage message: No Check routine interfaces: No

Compaq Visual Fortran 6.6	Intel Visual Fortran 11.1
	<p>OPTIMIZATION</p> <p>Optimization Diagnostic Level: Disable</p> <p>Emit Optimization Diagnostic to file: No</p> <p>Optimization Diagnostic File: blank</p> <p>Optimization Diagnostic Phase: All optimizer phases</p> <p>Optimization Diagnostic Routine: blank</p> <p>SOURCE CODE ANALYSIS</p> <p>Level of Source Code Analysis: None</p> <p>Level of source code parallelization: None</p> <p>Analyze include files: No</p>
DEBUG	DEBUGGING (diff title)
<p>Debugging Level: Full</p> <p>Compile DEBUG (D) lines: blank</p> <p>Use program database for Debug Information: checked</p> <p>Program Database (PDB) path: Debug/DF60.PDB</p> <p>Common Options: inheritance description not available</p>	<p>Debugging Level: Full (/debug:full)</p> <p>Enable Parallel Debug Checks: no</p> <p>Information for PARAMETER constants:None</p>
EXTERNAL PROCEDURES	EXTERNAL PROCEDURES
<p>Argument passing conventions: Default*</p> <p>External Names Interpretation: Upper case*</p> <p>String length argument passing: after string Arg*</p> <p>Append underscore to external names: not checked</p> <p>Common Options: inheritance description not available</p>	<p>Calling convention: Default</p> <p>Name Case interpretation: Default</p> <p>String length Argument passing: After all arguments</p> <p>Append Underscore to External names: No</p>
FLOATING POINT	FLOATING POINT
<p>Floating point exception handling: 3*</p> <p>Enable Floating point consistency: blank</p> <p>Extend Precision of single precision Constants: blank</p> <p>Enable IEEE Minus zero support</p>	<p>Floating-point exception handling: Produce NaN, signed infinities, and denormal results (/fpe:{0 1 3})</p> <p>Floating Point Model: Fast</p> <p>Reliable Floating Point Exceptions model: default</p> <p>Round Floating Point results: No</p> <p>Flush Denormal results to zero: No</p> <p>Extend precision of single precision constants: No</p> <p>Enable IEEE minus zero support: No</p> <p>Limit COMPLEX range: No</p> <p>Check Floating-Point Stack: No</p> <p>No</p> <p>Floating-point speculations: Safe</p>

Compaq Visual Fortran 6.6	Intel Visual Fortran 11.1
FORTTRAN DATA	DATA (diff title)
Default Real kind: 4 Default Integer kind: 4 Things checked: Constant actual arguments are read only Common Element alignment: 1* Structure element alignment: Natural*	Default Real kind: 4 Default Integer kind: 4 Default Double Precision kind: 8 Local variable storage: default Local storage Initialize local saved scalars to zero: no Dynamic common blocks: blank Structure element alignment: default Common Element alignment: None SEQUENCE types obey rules: no Assume summy argument share mememory : no Assume CRAY pointers do not share memory: no Constant actual arguments can be changed: no Use bytes as RECL= Unit for unformatted: no Initialize stack variables to an unusual value: no
FORTTRAN LANGUAGE	LANGUAGE (diff name)
Enable Fortran 66 semantics: blank Enable alternate PARAMETER syntax: checked Name interpretation : upper case* Source form: Use file extension* Fixed form line length: 72* Pad fixed form source records: blank	Source file format: Use file extension Fixed form line length: 72 columns Pad fixed form source records: no Enable alternate PARAMETER syntax: yes Enable Fortran 66 semantics: no Compile lines with D in column: no Process OpenMP Directives: disable
LIBRARIES	LIBRARIES
Reentrancy support: None Use run-time library: Debug Single-threaded* Other options checked: none	Use run-time library: Debug Multithreaded (/libs:static /threads /dbglibs) Use common windows libraries: No Use portlib library: No Use intel math kernel library: No Disable default library search Rules: No Disable OBJCOMMENT library names in object: No
LISTING FILES	OUTPUT FILES (diff name)
Source listing : blank Assembly listing: blank Common Options: inheritance description not available	Module path: \$(IntDir)\ Object File name: \$(IntDir)\ Assembler Output: No listing ASM listing name: \$(IntDir)\
OPTIMIZATIONS	OPTIMIZATIONS (2 nd in list here)

Compaq Visual Fortran 6.6	Intel Visual Fortran 11.1
Optimization level: None None selected in box Math library: Check* Loop unroll count: blank Inlining: blank Preprocessor to Optimize for: Blend*	Optimization: Disable (/Od) Inline Function Expansion: Disable Favor Size or Speed: Default Omit Frame pointers: No Loop unroll count: blank Parallelization: No Threshold for Auto=Parallelization: 100 Threshold for Vectorization: 100 Prefetch insertion: Disable I/O buffering: No Heap Arrays: blank Interprocedural Optimization: No
PREPROCESSOR	PREPROCESSOR
Predefined preprocessor symbols: blank Default INCLUDE and USE path: source directory* Module Path: blank INCLUDE and USE Paths: this is where we put the searchlist Use FPP: blank	Preprocess source file: No Additional include directories: blank Ignore standard include path: No Default INCLUDE and USE path: source file directory* Preprocessor definitions: blank Undefine Preprocessor definitions: blank Undefine All Preprocessor definitions: no Preprocessor definitions to FPP only: no OpenMP Conditional Compilation : yes
RUNTIME	RUNTIME
Generate Traceback information: checked Default output carriage control: default* Runtime error checking selected items: Array and string bounds Flawed Pentium processor Common Options: inheritance description not available	Generate Traceback information: yes (/traceback) Default output carriage control: default Runtime error checking: custom Check for null pointers and allocatable array refs: No Check Array and string bounds: yes (/check:bounds) Check uninitialized variables: no Check edit descriptor data type: no Check edit descriptor data size: no Check for actual arguments using temporary storage: no

The "Code Accumulation" method has the advantage of making compiling and linking very straight forward but the disadvantage that the source code is not directly traceable to the installed (archive) source directories.

Search List

When a "Search List" is used, there is no need to physically copy or move the source code. Instead links to the source code location are added to a Visual Fortran project. The recommended method is to only add the FORTRAN subroutines (*.FOR) and allow the INCLUDE files (*.INC) to be picked up by the compiler through the search list. This method does not actually move or copy the files but instead adds their location to a "Make" facility within the Visual Fortran environment.

The recommended search list for creation of the executable expects the executable to be built in, and source code to be installed in, the directory structure listed as follows:

```
..\..\Source\CC408\CCCODE\Inc\;..\..\Source\CC408\BTCODE\Inc\;  
..\..\Source\CC408\DOCODE\Inc\;..\..\Source\CC408\GTCODE\Inc\;  
..\..\Source\CC408\F3CODE\Inc\;..\..\Source\CC408\VTCODE\Inc\;  
..\..\Source\SV312\ECcode\Inc\;..\..\Source\SV312\FRcode\Inc\;  
..\..\Source\SV312\PScode\Inc\;..\..\Source\SV312\SVcode\Inc\;  
..\..\Source\SV312\TScode\Inc\;..\..\Source\ml303\ARcode\inc\;  
..\..\Source\ml303\FIcode\inc\/
```

where it may be noted that the ML303\SIcode and CC408\SLATEC do not appear in the latter search list since they do not have any INCLUDE files. For any duplicate FORTRAN modules, the CC4 version should be configured as the one that is actually compiled.

The use of a "Search List" has several advantages including:

- No need to make a temporary copy of all source code;
- "Make" file and other Visual Fortran project files reference the installed code areas;
- Only the required INCLUDE files are used, and they are referenced automatically without user intervention;
- Review of the source code can be done interactively through the Visual Fortran interface.

APPENDIX L: FRAC3DVS Input Files

This appendix shows the general format of a F3D*.FXD file and also shows the general format of a corresponding FRAC3DVS data file.

FRAC3DVS Control File Format

```
!
! F3D.FXD
!
! This file stores information needed for reading FRAC3DV output files
! The variables are stored in INCLUDE file F3DDAT.INC
!
! To change values, replace the existing values with new ones;
! To add more species labels/files, add new line(s) following
! the existing lines and use the same format
! Any modifications to this file structure or format are not allowed.
!
! 2003-AUG-05  VERSION 01A  K. WEI      CC404-F3D geosphere model
! 2004-JUN-23  VERSION 02C  T. MELNYK  CC405-F3D geosphere model
! 2004-JUL-19  VERSION 03A  L. WOJCIECHOWSKI  ** CNG05 testing
!
! 'TEST1'  ! ID for FRAC3DVS Run from which the data was obtained
!
! file names and species labels in FRAC3DVS
! and their corresponding NUCLID ID in SYVAC3:
!(unique part of file name only given, extension assumed to be .FXD
! and FRAC RUN ID assumed to be included)
! for example with Unique FILENAME ID 'nn', file F3D_xxx_nn.FXD is assumed)
! Unique FILENAME ID  SPECIES LABEL  NUCLIDE ID
!   '01'                1            'I 129 FUEL'
!& '02'                1            'U 238AFUEL'
!& '02'                2            'U 234AFUEL'
!& '02'                3            'TH234AFUEL'
!& '03'                1            'NP237AFUEL'
!& '03'                2            'U 233AFUEL'
!
! FRAC3DVS slice labels, indicator whether fluxes need sign reversal,
! and their corresponding discharge location indices in CC4,
! as numbered in SUBLABEL.GEO and NET.FXD
! FRAC3DVS slice label  Flip sign?  GEONET Discharge INDEX
!   'wel'                'YES'       1    ! well
!& 'lak'                'NO'        2    ! lake aqua
!& 'lak'                'NO'        3    ! lake terr
!& 'riv'                'NO'        4    ! river aqua
!& 'riv'                'NO'        5    ! river terr
!& 'str'                'NO'        6    ! stream aqua
!& 'str'                'NO'        7    ! stream
```

FRAC3DVS Data File Format

The following is an example of the contents of a file named F3D_xxx_nn.FXD, where xxx = run id and nn = the unique file name id. If the above control file was used for I-129, the file name would be F3D_TEST1_01.FXD. Note the file has been shortened to give an example of the fields in each line. All lines except for the first two start with a string label identifying the FRAC3DVS slice label. Each data line appears on two lines due to word wrapping.

```
!#Concentration and mass flux crossing slice output nodes
!slice sp time average_conc advective dispersive total cumulative_mass
'lak' 1 1000.00000 0.220171327E-290 0.219723322E-290 0.172644291E-288
0.174841524E-288 0.874207621E-286 0.874207621E-286
'riv' 1 1000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
'str' 1 1000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
'lak' 1 2000.00000 0.660514024E-290 0.659170008E-290 0.517932907E-288
0.524524607E-288 0.437103828E-285 0.349683065E-285
'riv' 1 2000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
'str' 1 2000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
'lak' 1 4000.00000 0.113499204E-279 0.566415701E-280 0.445015293E-278
0.450679450E-278 0.450679450E-275 0.450679450E-275
'riv' 1 4000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
'str' 1 4000.00000 0.000000000 0.000000000 0.000000000
0.000000000 0.000000000 0.000000000
...
'lak' 1 0.315576000E+014 0.237032685E-011 0.479138067E-016 0.485212303E-016
0.964350370E-016 0.698695278E-002 0.386087776E-004
'riv' 1 0.315576000E+014 0.906489339E-013 0.109419077E-015 0.393325273E-016
0.148751605E-015 0.187785007E-002 0.585943827E-004
'str' 1 0.315576000E+014 0.134860412E-020 0.142892824E-025 0.122490974E-025
0.265383798E-025 0.229419623E-012 0.102959800E-013
```